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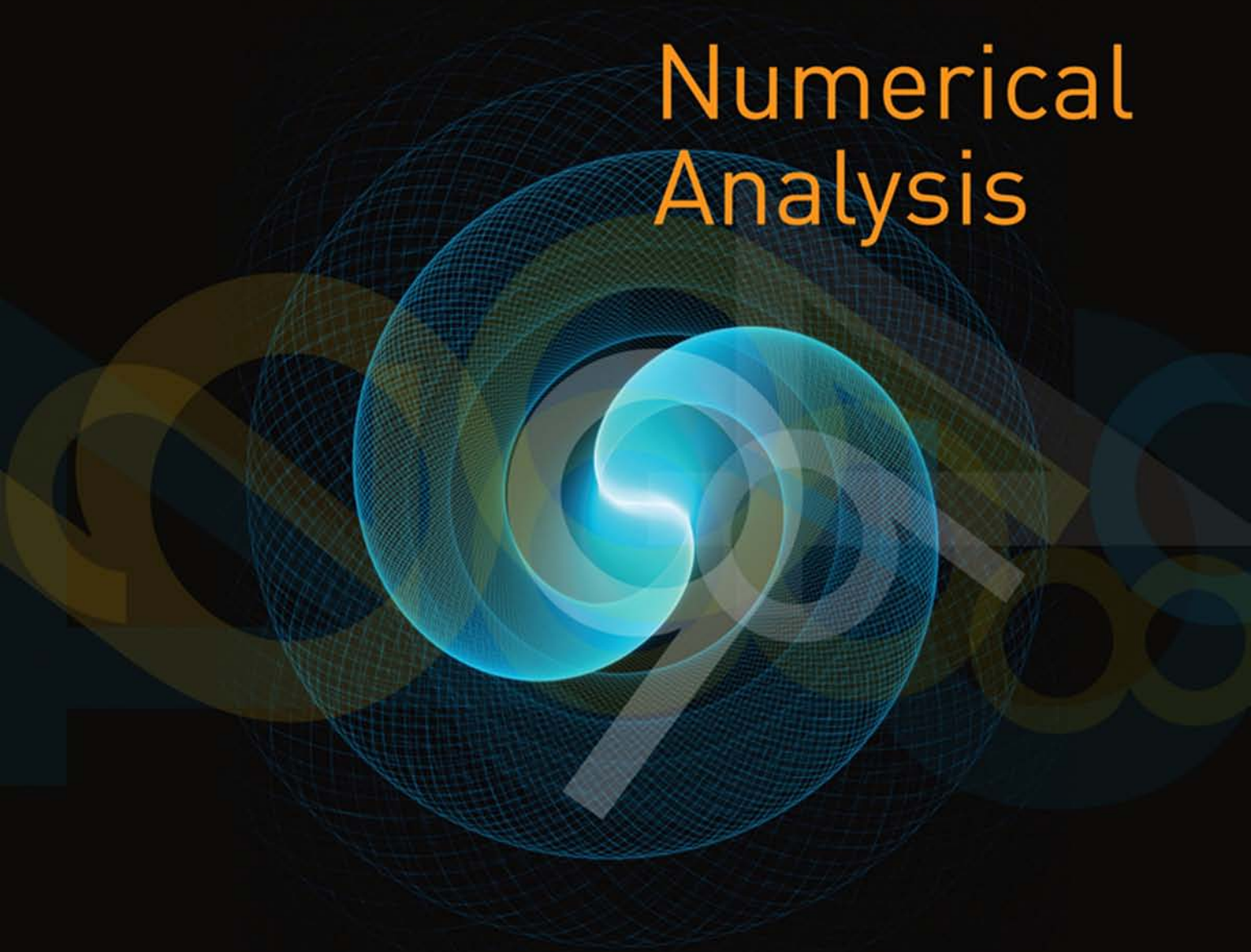
# Numerical Analysis



Ziyad Asaad

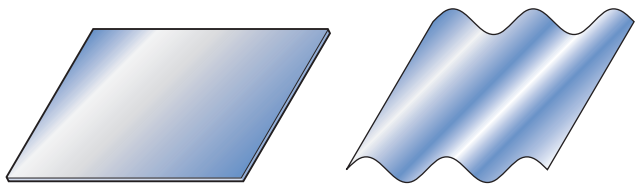
Ninth Edition

CHAPTER

# 4 Numerical Differentiation and Integration

## Introduction

A sheet of corrugated roofing is constructed by pressing a flat sheet of aluminum into one whose cross section has the form of a sine wave.



A corrugated sheet 4 ft long is needed, the height of each wave is 1 in. from the center line, and each wave has a period of approximately $2\pi$ in. The problem of finding the length of the initial flat sheet is one of determining the length of the curve given by $f(x) = \sin x$ from $x = 0$ in. to $x = 48$ in. From calculus we know that this length is

$$L = \int_0^{48} \sqrt{1 + (f'(x))^2}\, dx = \int_0^{48} \sqrt{1 + (\cos x)^2}\, dx,$$

so the problem reduces to evaluating this integral. Although the sine function is one of the most common mathematical functions, the calculation of its length involves an elliptic integral of the second kind, which cannot be evaluated explicitly. Methods are developed in this chapter to approximate the solution to problems of this type. This particular problem is considered in Exercise 25 of Section 4.4 and Exercise 12 of Section 4.5.

We mentioned in the introduction to Chapter 3 that one reason for using algebraic polynomials to approximate an arbitrary set of data is that, given any continuous function defined on a closed interval, there exists a polynomial that is arbitrarily close to the function at every point in the interval. Also, the derivatives and integrals of polynomials are easily obtained and evaluated. It should not be surprising, then, that many procedures for approximating derivatives and integrals use the polynomials that approximate the function.



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## 4.1 Numerical Differentiation

The derivative of the function $f$ at $x_0$ is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

This formula gives an obvious way to generate an approximation to $f'(x_0)$; simply compute

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of $h$. Although this may be obvious, it is not very successful, due to our old nemesis round-off error. But it is certainly a place to start.

To approximate $f'(x_0)$, suppose first that $x_0 \in (a, b)$, where $f \in C^2[a, b]$, and that $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a, b]$. We construct the first Lagrange polynomial $P_{0,1}(x)$ for $f$ determined by $x_0$ and $x_1$, with its error term:

$$\begin{aligned} f(x) &= P_{0,1}(x) + \frac{(x - x_0)(x - x_1)}{2!} f''(\xi(x)) \\ &= \frac{f(x_0)(x - x_0 - h)}{-h} + \frac{f(x_0 + h)(x - x_0)}{h} + \frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)), \end{aligned}$$

for some $\xi(x)$ between $x_0$ and $x_1$. Differentiating gives

$$\begin{aligned} f'(x) &= \frac{f(x_0 + h) - f(x_0)}{h} + D_x \left[ \frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)) \right] \\ &= \frac{f(x_0 + h) - f(x_0)}{h} + \frac{2(x - x_0) - h}{2} f''(\xi(x)) \\ &\quad + \frac{(x - x_0)(x - x_0 - h)}{2} D_x(f''(\xi(x))). \end{aligned}$$

Deleting the terms involving $\xi(x)$ gives

$$f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h}.$$

Difference equations were used and popularized by Isaac Newton in the last quarter of the 17th century, but many of these techniques had previously been developed by Thomas Harriot (1561–1621) and Henry Briggs (1561–1630). Harriot made significant advances in navigation techniques, and Briggs was the person most responsible for the acceptance of logarithms as an aid to computation.

One difficulty with this formula is that we have no information about $D_x f''(\xi(x))$, so the truncation error cannot be estimated. When $x$ is $x_0$, however, the coefficient of $D_x f''(\xi(x))$ is 0, and the formula simplifies to

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi). \tag{4.1}$$

For small values of $h$, the difference quotient $[f(x_0 + h) - f(x_0)]/h$ can be used to approximate $f'(x_0)$ with an error bounded by $M|h|/2$, where $M$ is a bound on $|f''(x)|$ for $x$ between $x_0$ and $x_0 + h$. This formula is known as the **forward-difference formula** if $h > 0$ (see Figure 4.1) and the **backward-difference formula** if $h < 0$.

**Example 1** Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, $h = 0.05$, and $h = 0.01$, and determine bounds for the approximation errors.

***Solution*** The forward-difference formula

$$\frac{f(1.8 + h) - f(1.8)}{h}$$

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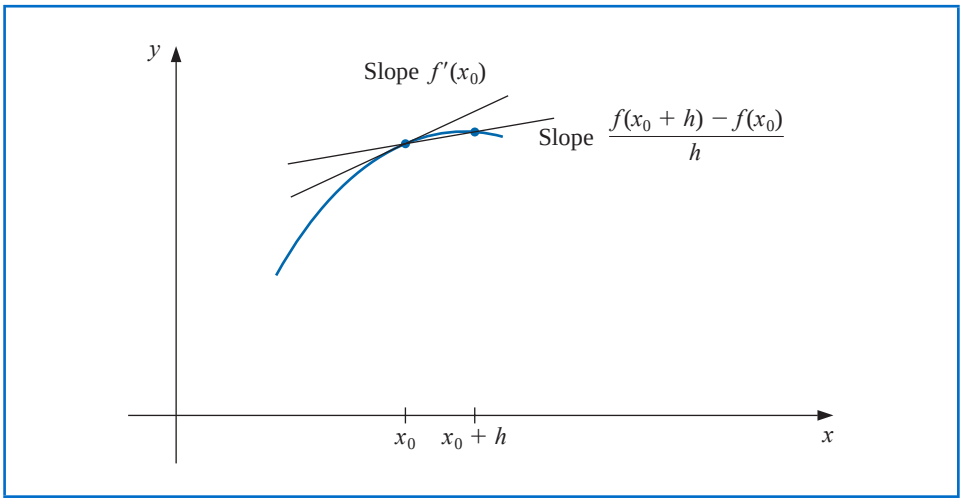
**Figure 4.1**




with $h = 0.1$ gives

$$\frac{\ln 1.9 - \ln 1.8}{0.1} = \frac{0.64185389 - 0.58778667}{0.1} = 0.5406722.$$

Because $f''(x) = -1/x^2$ and $1.8 < \xi < 1.9$, a bound for this approximation error is

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} < \frac{0.1}{2(1.8)^2} = 0.0154321.$$

The approximation and error bounds when $h = 0.05$ and $h = 0.01$ are found in a similar manner and the results are shown in Table 4.1.

**Table 4.1**

| $h$ | $f(1.8 + h)$ | $\frac{f(1.8 + h) - f(1.8)}{h}$ | $\frac{\lvert h\rvert}{2(1.8)^2}$ |
|---|---|---|---|
| 0.1 | 0.64185389 | 0.5406722 | 0.0154321 |
| 0.05 | 0.61518564 | 0.5479795 | 0.0077160 |
| 0.01 | 0.59332685 | 0.5540180 | 0.0015432 |

Since $f'(x) = 1/x$, the exact value of $f'(1.8)$ is $0.55\overline{5}$, and in this case the error bounds are quite close to the true approximation error. ■

To obtain general derivative approximation formulas, suppose that $\{x_0, x_1, \ldots, x_n\}$ are $(n + 1)$ distinct numbers in some interval $I$ and that $f \in C^{n+1}(I)$. From Theorem 3.3 on page 112,

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x - x_0)\cdots(x - x_n)}{(n + 1)!} f^{(n+1)}(\xi(x)),$$

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for some $\xi(x)$ in $I$, where $L_k(x)$ denotes the $k$th Lagrange coefficient polynomial for $f$ at $x_0, x_1, \ldots, x_n$. Differentiating this expression gives

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k'(x) + D_x\left[\frac{(x-x_0)\cdots(x-x_n)}{(n+1!)}\right] f^{(n+1)}(\xi(x)) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} D_x[f^{(n+1)}(\xi(x))].$$

We again have a problem estimating the truncation error unless $x$ is one of the numbers $x_j$. In this case, the term multiplying $D_x[f^{(n+1)}(\xi(x))]$ is 0, and the formula becomes

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0 \\ k\neq j}}^{n} (x_j - x_k), \tag{4.2}$$

which is called an **$(n+1)$-point formula** to approximate $f'(x_j)$.

In general, using more evaluation points in Eq. (4.2) produces greater accuracy, although the number of functional evaluations and growth of round-off error discourages this somewhat. The most common formulas are those involving three and five evaluation points.

We first derive some useful three-point formulas and consider aspects of their errors. Because

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad \text{we have} \quad L_0'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}.$$

Similarly,

$$L_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)} \quad \text{and} \quad L_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}.$$

Hence, from Eq. (4.2),

$$f'(x_j) = f(x_0)\left[\frac{2x_j-x_1-x_2}{(x_0-x_1)(x_0-x_2)}\right] + f(x_1)\left[\frac{2x_j-x_0-x_2}{(x_1-x_0)(x_1-x_2)}\right] + f(x_2)\left[\frac{2x_j-x_0-x_1}{(x_2-x_0)(x_2-x_1)}\right] + \frac{1}{6}f^{(3)}(\xi_j)\prod_{\substack{k=0 \\ k\neq j}}^{2}(x_j-x_k), \tag{4.3}$$

for each $j = 0, 1, 2$, where the notation $\xi_j$ indicates that this point depends on $x_j$.

## Three-Point Formulas

The formulas from Eq. (4.3) become especially useful if the nodes are equally spaced, that is, when

$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h, \quad \text{for some } h \neq 0.$$

We will assume equally-spaced nodes throughout the remainder of this section.

Using Eq. (4.3) with $x_j = x_0, x_1 = x_0 + h$, and $x_2 = x_0 + 2h$ gives

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_0).$$

Doing the same for $x_j = x_1$ gives

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

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and for $x_j = x_2$,

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, these formulas can also be expressed as

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0 + h) - \frac{1}{2}f(x_0 + 2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0 + h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0 + 2h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

and

$$f'(x_0 + 2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0 + h) + \frac{3}{2}f(x_0 + 2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

As a matter of convenience, the variable substitution $x_0$ for $x_0 + h$ is used in the middle equation to change this formula to an approximation for $f'(x_0)$. A similar change, $x_0$ for $x_0 + 2h$, is used in the last equation. This gives three formulas for approximating $f'(x_0)$:

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0) = \frac{1}{2h}[-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

and

$$f'(x_0) = \frac{1}{2h}[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

Finally, note that the last of these equations can be obtained from the first by simply replacing $h$ with $-h$, so there are actually only two formulas:

### Three-Point Endpoint Formula

- $$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0), \tag{4.4}$$

where $\xi_0$ lies between $x_0$ and $x_0 + 2h$.

### Three-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f^{(3)}(\xi_1), \tag{4.5}$$

where $\xi_1$ lies between $x_0 - h$ and $x_0 + h$.

Although the errors in both Eq. (4.4) and Eq. (4.5) are $O(h^2)$, the error in Eq. (4.5) is approximately half the error in Eq. (4.4). This is because Eq. (4.5) uses data on both sides of $x_0$ and Eq. (4.4) uses data on only one side. Note also that $f$ needs to be evaluated at only two points in Eq. (4.5), whereas in Eq. (4.4) three evaluations are needed. Figure 4.2 on page 178 gives an illustration of the approximation produced from Eq. (4.5). The approximation in Eq. (4.4) is useful near the ends of an interval, because information about $f$ outside the interval may not be available.

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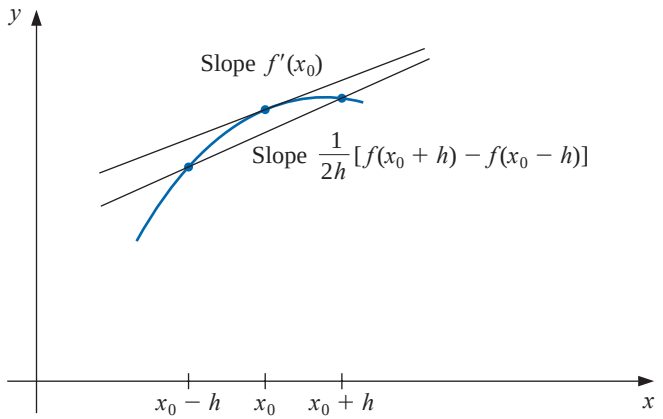
**Figure 4.2**




## Five-Point Formulas

The methods presented in Eqs. (4.4) and (4.5) are called **three-point formulas** (even though the third point $f(x_0)$ does not appear in Eq. (4.5)). Similarly, there are **five-point formulas** that involve evaluating the function at two additional points. The error term for these formulas is $O(h^4)$. One common five-point formula is used to determine approximations for the derivative at the midpoint.

## Five-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30}f^{(5)}(\xi), \tag{4.6}$$

  where $\xi$ lies between $x_0 - 2h$ and $x_0 + 2h$.

The derivation of this formula is considered in Section 4.2. The other five-point formula is used for approximations at the endpoints.

## Five-Point Endpoint Formula

- $$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5}f^{(5)}(\xi), \tag{4.7}$$

  where $\xi$ lies between $x_0$ and $x_0 + 4h$.

Left-endpoint approximations are found using this formula with $h > 0$ and right-endpoint approximations with $h < 0$. The five-point endpoint formula is particularly useful for the clamped cubic spline interpolation of Section 3.5.

**Example 2** Values for $f(x) = xe^x$ are given in Table 4.2. Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$.

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**Table 4.2**

| $x$ | $f(x)$ |
|---|---|
| 1.8 | 10.889365 |
| 1.9 | 12.703199 |
| 2.0 | 14.778112 |
| 2.1 | 17.148957 |
| 2.2 | 19.855030 |

***Solution*** The data in the table permit us to find four different three-point approximations. We can use the endpoint formula (4.4) with $h = 0.1$ or with $h = -0.1$, and we can use the midpoint formula (4.5) with $h = 0.1$ or with $h = 0.2$.

Using the endpoint formula (4.4) with $h = 0.1$ gives

$$\frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2] = 5[-3(14.778112) + 4(17.148957) - 19.855030)] = 22.032310,$$

and with $h = -0.1$ gives 22.054525.

Using the midpoint formula (4.5) with $h = 0.1$ gives

$$\frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.7703199) = 22.228790,$$

and with $h = 0.2$ gives 22.414163.

The only five-point formula for which the table gives sufficient data is the midpoint formula (4.6) with $h = 0.1$. This gives

$$\frac{1}{1.2}[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)] = \frac{1}{1.2}[10.889365 - 8(12.703199) + 8(17.148957) - 19.855030] = 22.166999$$

If we had no other information we would accept the five-point midpoint approximation using $h = 0.1$ as the most accurate, and expect the true value to be between that approximation and the three-point mid-point approximation that is in the interval [22.166, 22.229].

The true value in this case is $f'(2.0) = (2 + 1)e^2 = 22.167168$, so the approximation errors are actually:

Three-point endpoint with $h = 0.1$: $1.35 \times 10^{-1}$;

Three-point endpoint with $h = -0.1$: $1.13 \times 10^{-1}$;

Three-point midpoint with $h = 0.1$: $-6.16 \times 10^{-2}$;

Three-point midpoint with $h = 0.2$: $-2.47 \times 10^{-1}$;

Five-point midpoint with $h = 0.1$: $1.69 \times 10^{-4}$. ■

Methods can also be derived to find approximations to higher derivatives of a function using only tabulated values of the function at various points. The derivation is algebraically tedious, however, so only a representative procedure will be presented.

Expand a function $f$ in a third Taylor polynomial about a point $x_0$ and evaluate at $x_0 + h$ and $x_0 - h$. Then

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$

and

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4,$$

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

If we add these equations, the terms involving $f'(x_0)$ and $-f'(x_0)$ cancel, so

$$f(x_0 + h) + f(x_0 - h) = 2f(x_0) + f''(x_0)h^2 + \frac{1}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]h^4.$$

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Solving this equation for $f''(x_0)$ gives

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]. \qquad (4.8)$$

Suppose $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$. Since $\frac{1}{2}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the Intermediate Value Theorem implies that a number $\xi$ exists between $\xi_1$ and $\xi_{-1}$, and hence in $(x_0 - h, x_0 + h)$, with

$$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right].$$

This permits us to rewrite Eq. (4.8) in its final form.

## Second Derivative Midpoint Formula

- $$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12}f^{(4)}(\xi), \qquad (4.9)$$

  for some $\xi$, where $x_0 - h < \xi < x_0 + h$.

If $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$ it is also bounded, and the approximation is $O(h^2)$.

**Example 3** In Example 2 we used the data shown in Table 4.3 to approximate the first derivative of $f(x) = xe^x$ at $x = 2.0$. Use the second derivative formula (4.9) to approximate $f''(2.0)$.

**Table 4.3**

| $x$ | $f(x)$ |
|---|---|
| 1.8 | 10.889365 |
| 1.9 | 12.703199 |
| 2.0 | 14.778112 |
| 2.1 | 17.148957 |
| 2.2 | 19.855030 |

***Solution*** The data permits us to determine two approximations for $f''(2.0)$. Using (4.9) with $h = 0.1$ gives

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)] = 100[12.703199 - 2(14.778112) + 17.148957]$$
$$= 29.593200,$$

and using (4.9) with $h = 0.2$ gives

$$\frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)] = 25[10.889365 - 2(14.778112) + 19.855030]$$
$$= 29.704275.$$

Because $f''(x) = (x + 2)e^x$, the exact value is $f''(2.0) = 29.556224$. Hence the actual errors are $-3.70 \times 10^{-2}$ and $-1.48 \times 10^{-1}$, respectively. ■

## Round-Off Error Instability

It is particularly important to pay attention to round-off error when approximating derivatives. To illustrate the situation, let us examine the three-point midpoint formula Eq. (4.5),

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

more closely. Suppose that in evaluating $f(x_0 + h)$ and $f(x_0 - h)$ we encounter round-off errors $e(x_0 + h)$ and $e(x_0 - h)$. Then our computations actually use the values $\tilde{f}(x_0 + h)$ and $\tilde{f}(x_0 - h)$, which are related to the true values $f(x_0 + h)$ and $f(x_0 - h)$ by

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$$f(x_0 + h) = \tilde{f}(x_0 + h) + e(x_0 + h) \quad \text{and} \quad f(x_0 - h) = \tilde{f}(x_0 - h) + e(x_0 - h).$$

The total error in the approximation,

$$f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} = \frac{e(x_0 + h) - e(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1),$$

is due both to round-off error, the first part, and to truncation error. If we assume that the round-off errors $e(x_0 \pm h)$ are bounded by some number $\varepsilon > 0$ and that the third derivative of $f$ is bounded by a number $M > 0$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2}{6} M.$$

To reduce the truncation error, $h^2M/6$, we need to reduce $h$. But as $h$ is reduced, the round-off error $\varepsilon/h$ grows. In practice, then, it is seldom advantageous to let $h$ be too small, because in that case the round-off error will dominate the calculations.

**Illustration** Consider using the values in Table 4.4 to approximate $f'(0.900)$, where $f(x) = \sin x$. The true value is $\cos 0.900 = 0.62161$. The formula

$$f'(0.900) \approx \frac{f(0.900 + h) - f(0.900 - h)}{2h},$$

with different values of $h$, gives the approximations in Table 4.5.

**Table 4.4**

| $x$ | $\sin x$ | $x$ | $\sin x$ |
|---|---|---|---|
| 0.800 | 0.71736 | 0.901 | 0.78395 |
| 0.850 | 0.75128 | 0.902 | 0.78457 |
| 0.880 | 0.77074 | 0.905 | 0.78643 |
| 0.890 | 0.77707 | 0.910 | 0.78950 |
| 0.895 | 0.78021 | 0.920 | 0.79560 |
| 0.898 | 0.78208 | 0.950 | 0.81342 |
| 0.899 | 0.78270 | 1.000 | 0.84147 |

**Table 4.5**

| $h$ | Approximation to $f'(0.900)$ | Error |
|---|---|---|
| 0.001 | 0.62500 | 0.00339 |
| 0.002 | 0.62250 | 0.00089 |
| 0.005 | 0.62200 | 0.00039 |
| 0.010 | 0.62150 | −0.00011 |
| 0.020 | 0.62150 | −0.00011 |
| 0.050 | 0.62140 | −0.00021 |
| 0.100 | 0.62055 | −0.00106 |

The optimal choice for $h$ appears to lie between 0.005 and 0.05. We can use calculus to verify (see Exercise 29) that a minimum for

$$e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6} M,$$

occurs at $h = \sqrt[3]{3\varepsilon/M}$, where

$$M = \max_{x \in [0.800, 1.00]} |f'''(x)| = \max_{x \in [0.800, 1.00]} |\cos x| = \cos 0.8 \approx 0.69671.$$

Because values of $f$ are given to five decimal places, we will assume that the round-off error is bounded by $\varepsilon = 5 \times 10^{-6}$. Therefore, the optimal choice of $h$ is approximately

$$h = \sqrt[3]{\frac{3(0.000005)}{0.69671}} \approx 0.028,$$

which is consistent with the results in Table 4.6. □

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In practice, we cannot compute an optimal $h$ to use in approximating the derivative, since we have no knowledge of the third derivative of the function. But we must remain aware that reducing the step size will not always improve the approximation. □

We have considered only the round-off error problems that are presented by the three-point formula Eq. (4.5), but similar difficulties occur with all the differentiation formulas. The reason can be traced to the need to divide by a power of $h$. As we found in Section 1.2 (see, in particular, Example 3), division by small numbers tends to exaggerate round-off error, and this operation should be avoided if possible. In the case of numerical differentiation, we cannot avoid the problem entirely, although the higher-order methods reduce the difficulty.

Keep in mind that difference method approximations might be unstable.

As approximation methods, numerical differentiation is *unstable*, since the small values of $h$ needed to reduce truncation error also cause the round-off error to grow. This is the first class of unstable methods we have encountered, and these techniques would be avoided if it were possible. However, in addition to being used for computational purposes, the formulas are needed for approximating the solutions of ordinary and partial-differential equations.

## EXERCISE SET 4.1

**1.** Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables.

**a.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 0.5 | 0.4794 | |
| 0.6 | 0.5646 | |
| 0.7 | 0.6442 | |

**b.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 0.0 | 0.00000 | |
| 0.2 | 0.74140 | |
| 0.4 | 1.3718 | |

**2.** Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables.

**a.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| −0.3 | 1.9507 | |
| −0.2 | 2.0421 | |
| −0.1 | 2.0601 | |

**b.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 1.0 | 1.0000 | |
| 1.2 | 1.2625 | |
| 1.4 | 1.6595 | |

**3.** The data in Exercise 1 were taken from the following functions. Compute the actual errors in Exercise 1, and find error bounds using the error formulas.

**a.** $f(x) = \sin x$ **b.** $f(x) = e^x - 2x^2 + 3x - 1$

**4.** The data in Exercise 2 were taken from the following functions. Compute the actual errors in Exercise 2, and find error bounds using the error formulas.

**a.** $f(x) = 2\cos 2x - x$ **b.** $f(x) = x^2 \ln x + 1$

**5.** Use the most accurate three-point formula to determine each missing entry in the following tables.

**a.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 1.1 | 9.025013 | |
| 1.2 | 11.02318 | |
| 1.3 | 13.46374 | |
| 1.4 | 16.44465 | |

**b.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 8.1 | 16.94410 | |
| 8.3 | 17.56492 | |
| 8.5 | 18.19056 | |
| 8.7 | 18.82091 | |

**c.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 2.9 | −4.827866 | |
| 3.0 | −4.240058 | |
| 3.1 | −3.496909 | |
| 3.2 | −2.596792 | |

**d.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 2.0 | 3.6887983 | |
| 2.1 | 3.6905701 | |
| 2.2 | 3.6688192 | |
| 2.3 | 3.6245909 | |

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**6.** Use the most accurate three-point formula to determine each missing entry in the following tables.

**a.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| −0.3 | −0.27652 | |
| −0.2 | −0.25074 | |
| −0.1 | −0.16134 | |
| 0 | 0 | |

**b.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 7.4 | −68.3193 | |
| 7.6 | −71.6982 | |
| 7.8 | −75.1576 | |
| 8.0 | −78.6974 | |

**c.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 1.1 | 1.52918 | |
| 1.2 | 1.64024 | |
| 1.3 | 1.70470 | |
| 1.4 | 1.71277 | |

**d.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| −2.7 | 0.054797 | |
| −2.5 | 0.11342 | |
| −2.3 | 0.65536 | |
| −2.1 | 0.98472 | |

**7.** The data in Exercise 5 were taken from the following functions. Compute the actual errors in Exercise 5, and find error bounds using the error formulas.

**a.** $f(x) = e^{2x}$ **b.** $f(x) = x \ln x$

**c.** $f(x) = x \cos x - x^2 \sin x$ **d.** $f(x) = 2(\ln x)^2 + 3 \sin x$

**8.** The data in Exercise 6 were taken from the following functions. Compute the actual errors in Exercise 6, and find error bounds using the error formulas.

**a.** $f(x) = e^{2x} - \cos 2x$ **b.** $f(x) = \ln(x+2) - (x+1)^2$

**c.** $f(x) = x \sin x + x^2 \cos x$ **d.** $f(x) = (\cos 3x)^2 - e^{2x}$

**9.** Use the formulas given in this section to determine, as accurately as possible, approximations for each missing entry in the following tables.

**a.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 2.1 | −1.709847 | |
| 2.2 | −1.373823 | |
| 2.3 | −1.119214 | |
| 2.4 | −0.9160143 | |
| 2.5 | −0.7470223 | |
| 2.6 | −0.6015966 | |

**b.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| −3.0 | 9.367879 | |
| −2.8 | 8.233241 | |
| −2.6 | 7.180350 | |
| −2.4 | 6.209329 | |
| −2.2 | 5.320305 | |
| −2.0 | 4.513417 | |

**10.** Use the formulas given in this section to determine, as accurately as possible, approximations for each missing entry in the following tables.

**a.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| 1.05 | −1.709847 | |
| 1.10 | −1.373823 | |
| 1.15 | −1.119214 | |
| 1.20 | −0.9160143 | |
| 1.25 | −0.7470223 | |
| 1.30 | −0.6015966 | |

**b.**

| $x$ | $f(x)$ | $f'(x)$ |
|---|---|---|
| −3.0 | 16.08554 | |
| −2.8 | 12.64465 | |
| −2.6 | 9.863738 | |
| −2.4 | 7.623176 | |
| −2.2 | 5.825013 | |
| −2.0 | 4.389056 | |

**11.** The data in Exercise 9 were taken from the following functions. Compute the actual errors in Exercise 9, and find error bounds using the error formulas and Maple.

**a.** $f(x) = \tan x$ **b.** $f(x) = e^{x/3} + x^2$

**12.** The data in Exercise 10 were taken from the following functions. Compute the actual errors in Exercise 10, and find error bounds using the error formulas and Maple.

**a.** $f(x) = \tan 2x$ **b.** $f(x) = e^{-x} - 1 + x$

**13.** Use the following data and the knowledge that the first five derivatives of $f$ are bounded on $[1, 5]$ by 2, 3, 6, 12 and 23, respectively, to approximate $f'(3)$ as accurately as possible. Find a bound for the error.

| $x$ | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| $f(x)$ | 2.4142 | 2.6734 | 2.8974 | 3.0976 | 3.2804 |

**14.** Repeat Exercise 13, assuming instead that the third derivative of $f$ is bounded on $[1, 5]$ by 4.

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**15.** Repeat Exercise 1 using four-digit rounding arithmetic, and compare the errors to those in Exercise 3.

**16.** Repeat Exercise 5 using four-digit chopping arithmetic, and compare the errors to those in Exercise 7.

**17.** Repeat Exercise 9 using four-digit rounding arithmetic, and compare the errors to those in Exercise 11.

**18.** Consider the following table of data:

| $x$ | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
|---|---|---|---|---|---|
| $f(x)$ | 0.9798652 | 0.9177710 | 0.808038 | 0.6386093 | 0.3843735 |

**a.** Use all the appropriate formulas given in this section to approximate $f'(0.4)$ and $f''(0.4)$.

**b.** Use all the appropriate formulas given in this section to approximate $f'(0.6)$ and $f''(0.6)$.

**19.** Let $f(x) = \cos \pi x$. Use Eq. (4.9) and the values of $f(x)$ at $x = 0.25$, 0.5, and 0.75 to approximate $f''(0.5)$. Compare this result to the exact value and to the approximation found in Exercise 15 of Section 3.5. Explain why this method is particularly accurate for this problem, and find a bound for the error.

**20.** Let $f(x) = 3xe^x - \cos x$. Use the following data and Eq. (4.9) to approximate $f''(1.3)$ with $h = 0.1$ and with $h = 0.01$.

| $x$ | 1.20 | 1.29 | 1.30 | 1.31 | 1.40 |
|---|---|---|---|---|---|
| $f(x)$ | 11.59006 | 13.78176 | 14.04276 | 14.30741 | 16.86187 |

Compare your results to $f''(1.3)$.

**21.** Consider the following table of data:

| $x$ | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |
|---|---|---|---|---|---|
| $f(x)$ | 0.9798652 | 0.9177710 | 0.8080348 | 0.6386093 | 0.3843735 |

**a.** Use Eq. (4.7) to approximate $f'(0.2)$.

**b.** Use Eq. (4.7) to approximate $f'(1.0)$.

**c.** Use Eq. (4.6) to approximate $f'(0.6)$.

**22.** Derive an $O(h^4)$ five-point formula to approximate $f'(x_0)$ that uses $f(x_0 - h)$, $f(x_0)$, $f(x_0 + h)$, $f(x_0 + 2h)$, and $f(x_0 + 3h)$. [*Hint:* Consider the expression $Af(x_0 - h) + Bf(x_0 + h) + Cf(x_0 + 2h) + Df(x_0 + 3h)$. Expand in fourth Taylor polynomials, and choose $A, B, C$, and $D$ appropriately.]

**23.** Use the formula derived in Exercise 22 and the data of Exercise 21 to approximate $f'(0.4)$ and $f'(0.8)$.

**24.** **a.** Analyze the round-off errors, as in Example 4, for the formula

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi_0).$$

**b.** Find an optimal $h > 0$ for the function given in Example 2.

**25.** In Exercise 10 of Section 3.4 data were given describing a car traveling on a straight road. That problem asked to predict the position and speed of the car when $t = 10$ s. Use the following times and positions to predict the speed at each time listed.

| Time | 0 | 3 | 5 | 8 | 10 | 13 |
|---|---|---|---|---|---|---|
| Distance | 0 | 225 | 383 | 623 | 742 | 993 |

**26.** In a circuit with impressed voltage $\mathcal{E}(t)$ and inductance $L$, Kirchhoff's first law gives the relationship

$$\mathcal{E}(t) = L\frac{di}{dt} + Ri,$$

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where $R$ is the resistance in the circuit and $i$ is the current. Suppose we measure the current for several values of $t$ and obtain:

| $t$ | 1.00 | 1.01 | 1.02 | 1.03 | 1.0 |
|---|---|---|---|---|---|
| $i$ | 3.10 | 3.12 | 3.14 | 3.18 | 3.24 |

where $t$ is measured in seconds, $i$ is in amperes, the inductance $L$ is a constant 0.98 henries, and the resistance is 0.142 ohms. Approximate the voltage $\mathcal{E}(t)$ when $t = 1.00, 1.01, 1.02, 1.03$, and $1.04$.

**27.** All calculus students know that the derivative of a function $f$ at $x$ can be defined as

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

Choose your favorite function $f$, nonzero number $x$, and computer or calculator. Generate approximations $f_n'(x)$ to $f'(x)$ by

$$f_n'(x) = \frac{f(x + 10^{-n}) - f(x)}{10^{-n}},$$

for $n = 1, 2, \ldots, 20$, and describe what happens.

**28.** Derive a method for approximating $f''''(x_0)$ whose error term is of order $h^2$ by expanding the function $f$ in a fourth Taylor polynomial about $x_0$ and evaluating at $x_0 \pm h$ and $x_0 \pm 2h$.

**29.** Consider the function

$$e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6}M,$$

where $M$ is a bound for the third derivative of a function. Show that $e(h)$ has a minimum at $\sqrt[3]{3\varepsilon/M}$.

## 4.2 Richardson's Extrapolation

Lewis Fry Richardson (1881–1953) was the first person to systematically apply mathematics to weather prediction while working in England for the Meteorological Office. As a conscientious objector during World War I, he wrote extensively about the economic futility of warfare, using systems of differential equations to model rational interactions between countries. The extrapolation technique that bears his name was the rediscovery of a technique with roots that are at least as old as Christiaan Hugyens (1629–1695), and possibly Archimedes (287–212 B.C.E.).

Richardson's extrapolation is used to generate high-accuracy results while using low-order formulas. Although the name attached to the method refers to a paper written by L. F. Richardson and J. A. Gaunt [RG] in 1927, the idea behind the technique is much older. An interesting article regarding the history and application of extrapolation can be found in [Joy].

Extrapolation can be applied whenever it is known that an approximation technique has an error term with a predictable form, one that depends on a parameter, usually the step size $h$. Suppose that for each number $h \neq 0$ we have a formula $N_1(h)$ that approximates an unknown constant $M$, and that the truncation error involved with the approximation has the form

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots,$$

for some collection of (unknown) constants $K_1, K_2, K_3, \ldots$.

The truncation error is $O(h)$, so unless there was a large variation in magnitude among the constants $K_1, K_2, K_3, \ldots$,

$$M - N_1(0.1) \approx 0.1K_1, \quad M - N_1(0.01) \approx 0.01K_1,$$

and, in general, $M - N_1(h) \approx K_1 h$.

The object of extrapolation is to find an easy way to combine these rather inaccurate $O(h)$ approximations in an appropriate way to produce formulas with a higher-order truncation error.

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Suppose, for example, we can combine the $N_1(h)$ formulas to produce an $O(h^2)$ approximation formula, $N_2(h)$, for $M$ with

$$M - N_2(h) = \hat{K}_2 h^2 + \hat{K}_3 h^3 + \cdots,$$

for some, again unknown, collection of constants $\hat{K}_2, \hat{K}_3, \ldots$. Then we would have

$$M - N_2(0.1) \approx 0.01\hat{K}_2, \quad M - N_2(0.01) \approx 0.0001\hat{K}_2,$$

and so on. If the constants $K_1$ and $\hat{K}_2$ are roughly of the same magnitude, then the $N_2(h)$ approximations would be much better than the corresponding $N_1(h)$ approximations. The extrapolation continues by combining the $N_2(h)$ approximations in a manner that produces formulas with $O(h^3)$ truncation error, and so on.

To see specifically how we can generate the extrapolation formulas, consider the $O(h)$ formula for approximating $M$

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots. \tag{4.10}$$

The formula is assumed to hold for all positive $h$, so we replace the parameter $h$ by half its value. Then we have a second $O(h)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h}{2} + K_2\frac{h^2}{4} + K_3\frac{h^3}{8} + \cdots. \tag{4.11}$$

Subtracting Eq. (4.10) from twice Eq. (4.11) eliminates the term involving $K_1$ and gives

$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots. \tag{4.12}$$

Define

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right].$$

Then Eq. (4.12) is an $O(h^2)$ approximation formula for $M$:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots. \tag{4.13}$$

**Example 1** In Example 1 of Section 4.1 we use the forward-difference method with $h = 0.1$ and $h = 0.05$ to find approximations to $f'(1.8)$ for $f(x) = \ln(x)$. Assume that this formula has truncation error $O(h)$ and use extrapolation on these values to see if this results in a better approximation.

***Solution*** In Example 1 of Section 4.1 we found that

$$\text{with } h = 0.1\text{: } f'(1.8) \approx 0.5406722, \quad \text{and} \quad \text{with } h = 0.05\text{: } f'(1.8) \approx 0.5479795.$$

This implies that

$$N_1(0.1) = 0.5406722 \quad \text{and} \quad N_1(0.05) = 0.5479795.$$

Extrapolating these results gives the new approximation

$$N_2(0.1) = N_1(0.05) + (N_1(0.05) - N_1(0.1)) = 0.5479795 + (0.5479795 - 0.5406722)$$
$$= 0.555287.$$

The $h = 0.1$ and $h = 0.05$ results were found to be accurate to within $1.5 \times 10^{-2}$ and $7.7 \times 10^{-3}$, respectively. Because $f'(1.8) = 1/1.8 = 0.\overline{5}$, the extrapolated value is accurate to within $2.7 \times 10^{-4}$. ■

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Extrapolation can be applied whenever the truncation error for a formula has the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m}),$$

for a collection of constants $K_j$ and when $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$. Many formulas used for extrapolation have truncation errors that contain only even powers of $h$, that is, have the form

$$M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots . \tag{4.14}$$

The extrapolation is much more effective than when all powers of $h$ are present because the averaging process produces results with errors $O(h^2)$, $O(h^4)$, $O(h^6)$, ..., with essentially no increase in computation, over the results with errors, $O(h)$, $O(h^2)$, $O(h^3)$, ....

Assume that approximation has the form of Eq. (4.14 ). Replacing $h$ with $h/2$ gives the $O(h^2)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h^2}{4} + K_2\frac{h^4}{16} + K_3\frac{h^6}{64} + \cdots .$$

Subtracting Eq. (4.14) from 4 times this equation eliminates the $h^2$ term,

$$3M = \left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^4}{4} - h^4\right) + K_3\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Dividing this equation by 3 produces an $O(h^4)$ formula

$$M = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + \frac{K_2}{3}\left(\frac{h^4}{4} - h^4\right) + \frac{K_3}{3}\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Defining

$$N_2(h) = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] = N_1\left(\frac{h}{2}\right) + \frac{1}{3}\left[N_1\left(\frac{h}{2}\right) - N_1(h)\right],$$

produces the approximation formula with truncation error $O(h^4)$:

$$M = N_2(h) - K_2\frac{h^4}{4} - K_3\frac{5h^6}{16} + \cdots . \tag{4.15}$$

Now replace $h$ in Eq. (4.15) with $h/2$ to produce a second $O(h^4)$ formula

$$M = N_2\left(\frac{h}{2}\right) - K_2\frac{h^4}{64} - K_3\frac{5h^6}{1024} - \cdots .$$

Subtracting Eq. (4.15 ) from 16 times this equation eliminates the $h^4$ term and gives

$$15M = \left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{15h^6}{64} + \cdots .$$

Dividing this equation by 15 produces the new $O(h^6)$ formula

$$M = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{h^6}{64} + \cdots .$$

We now have the $O(h^6)$ approximation formula

$$N_3(h) = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] = N_2\left(\frac{h}{2}\right) + \frac{1}{15}\left[N_2\left(\frac{h}{2}\right) - N_2(h)\right].$$

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Continuing this procedure gives, for each $j = 2, 3, \ldots$, the $O(h^{2j})$ approximation

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}.$$

Table 4.6 shows the order in which the approximations are generated when

$$M = N_1(h) + K_1h^2 + K_2h^4 + K_3h^6 + \cdots. \tag{4.16}$$

It is conservatively assumed that the true result is accurate at least to within the agreement of the bottom two results in the diagonal, in this case, to within $|N_3(h) - N_4(h)|$.

**Table 4.6**

| $O(h^2)$ | $O(h^4)$ | $O(h^6)$ | $O(h^8)$ |
|---|---|---|---|
| **1:** $N_1(h)$ | | | |
| **2:** $N_1(\frac{h}{2})$ | **3:** $N_2(h)$ | | |
| **4:** $N_1(\frac{h}{4})$ | **5:** $N_2(\frac{h}{2})$ | **6:** $N_3(h)$ | |
| **7:** $N_1(\frac{h}{8})$ | **8:** $N_2(\frac{h}{4})$ | **9:** $N_3(\frac{h}{2})$ | **10:** $N_4(h)$ |

**Example 2** Taylor's theorem can be used to show that centered-difference formula in Eq. (4.5) to approximate $f'(x_0)$ can be expressed with an error formula:

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots.$$

Find approximations of order $O(h^2)$, $O(h^4)$, and $O(h^6)$ for $f'(2.0)$ when $f(x) = xe^x$ and $h = 0.2$.

***Solution*** The constants $K_1 = -f'''(x_0)/6$, $K_2 = -f^{(5)}(x_0)/120, \cdots$, are not likely to be known, but this is not important. We only need to know that these constants exist in order to apply extrapolation.

We have the $O(h^2)$ approximation

$$f'(x_0) = N_1(h) - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots, \tag{4.17}$$

where

$$N_1(h) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)].$$

This gives us the first $O(h^2)$ approximations

$$N_1(0.2) = \frac{1}{0.4}[f(2.2) - f(1.8)] = 2.5(19.855030 - 10.889365) = 22.414160,$$

and

$$N_1(0.1) = \frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.703199) = 22.228786.$$

Combining these to produce the first $O(h^4)$ approximation gives

$$\begin{aligned} N_2(0.2) &= N_1(0.1) + \frac{1}{3}(N_1(0.1) - N_1(0.2)) \\ &= 22.228786 + \frac{1}{3}(22.228786 - 22.414160) = 22.166995. \end{aligned}$$

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To determine an $O(h^6)$ formula we need another $O(h^4)$ result, which requires us to find the third $O(h^2)$ approximation

$$N_1(0.05) = \frac{1}{0.1}[f(2.05) - f(1.95)] = 10(15.924197 - 13.705941) = 22.182564.$$

We can now find the $O(h^4)$ approximation

$$\begin{aligned} N_2(0.1) &= N_1(0.05) + \frac{1}{3}(N_1(0.05) - N_1(0.1)) \\ &= 22.182564 + \frac{1}{3}(22.182564 - 22.228786) = 22.167157. \end{aligned}$$

and finally the $O(h^6)$ approximation

$$\begin{aligned} N_3(0.2) &= N_2(0.1) + \frac{1}{15}(N_2(0.1) - N_1(0.2)) \\ &= 22.167157 + \frac{1}{15}(22.167157 - 22.166995) = 22.167168. \end{aligned}$$

We would expect the final approximation to be accurate to at least the value 22.167 because the $N_2(0.2)$ and $N_3(0.2)$ give this same value. In fact, $N_3(0.2)$ is accurate to all the listed digits. ■

Each column beyond the first in the extrapolation table is obtained by a simple averaging process, so the technique can produce high-order approximations with minimal computational cost. However, as $k$ increases, the round-off error in $N_1(h/2^k)$ will generally increase because the instability of numerical differentiation is related to the step size $h/2^k$. Also, the higher-order formulas depend increasingly on the entry to their immediate left in the table, which is the reason we recommend comparing the final diagonal entries to ensure accuracy.

In Section 4.1, we discussed both three- and five-point methods for approximating $f'(x_0)$ given various functional values of $f$. The three-point methods were derived by differentiating a Lagrange interpolating polynomial for $f$. The five-point methods can be obtained in a similar manner, but the derivation is tedious. Extrapolation can be used to more easily derive these formulas, as illustrated below.

**Illustration** Suppose we expand the function $f$ in a fourth Taylor polynomial about $x_0$. Then

$$\begin{aligned} f(x) = &f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 + \frac{1}{6}f'''(x_0)(x - x_0)^3 \\ &+ \frac{1}{24}f^{(4)}(x_0)(x - x_0)^4 + \frac{1}{120}f^{(5)}(\xi)(x - x_0)^5, \end{aligned}$$

for some number $\xi$ between $x$ and $x_0$. Evaluating $f$ at $x_0 + h$ and $x_0 - h$ gives

$$\begin{aligned} f(x_0 + h) = &f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 \\ &+ \frac{1}{24}f^{(4)}(x_0)h^4 + \frac{1}{120}f^{(5)}(\xi_1)h^5 \end{aligned} \tag{4.18}$$

and

$$\begin{aligned} f(x_0 - h) = &f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 \\ &+ \frac{1}{24}f^{(4)}(x_0)h^4 - \frac{1}{120}f^{(5)}(\xi_2)h^5, \end{aligned} \tag{4.19}$$

where $x_0 - h < \xi_2 < x_0 < \xi_1 < x_0 + h$.

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Subtracting Eq. (4.19) from Eq. (4.18) gives a new approximation for $f'(x)$.

$$f(x_0 + h) - f(x_0 - h) = 2hf'(x_0) + \frac{h^3}{3}f'''(x_0) + \frac{h^5}{120}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)], \quad (4.20)$$

which implies that

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{240}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)].$$

If $f^{(5)}$ is continuous on $[x_0 - h, x_0 + h]$, the Intermediate Value Theorem 1.11 implies that a number $\tilde{\xi}$ in $(x_0 - h, x_0 + h)$ exists with

$$f^{(5)}(\tilde{\xi}) = \frac{1}{2}\left[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)\right].$$

As a consequence,we have the $O(h^2)$ approximation

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(\tilde{\xi}). \quad (4.21)$$

Although the approximation in Eq. (4.21) is the same as that given in the three-point formula in Eq. (4.5), the unknown evaluation point occurs now in $f^{(5)}$, rather than in $f'''$. Extrapolation takes advantage of this by first replacing $h$ in Eq. (4.21) with $2h$ to give the new formula

$$f'(x_0) = \frac{1}{4h}[f(x_0 + 2h) - f(x_0 - 2h)] - \frac{4h^2}{6}f'''(x_0) - \frac{16h^4}{120}f^{(5)}(\hat{\xi}), \quad (4.22)$$

where $\hat{\xi}$ is between $x_0 - 2h$ and $x_0 + 2h$.

Multiplying Eq. (4.21) by 4 and subtracting Eq. (4.22) produces

$$3f'(x_0) = \frac{2}{h}[f(x_0 + h) - f(x_0 - h)] - \frac{1}{4h}[f(x_0 + 2h) - f(x_0 - 2h)] - \frac{h^4}{30}f^{(5)}(\tilde{\xi}) + \frac{2h^4}{15}f^{(5)}(\hat{\xi}).$$

Even if $f^{(5)}$ is continuous on $[x_0 - 2h, x_0 + 2h]$, the Intermediate Value Theorem 1.11 cannot be applied as we did to derive Eq. (4.21) because here we have the *difference* of terms involving $f^{(5)}$. However, an alternative method can be used to show that $f^{(5)}(\tilde{\xi})$ and $f^{(5)}(\hat{\xi})$ can still be replaced by a common value $f^{(5)}(\xi)$. Assuming this and dividing by 3 produces the five-point midpoint formula Eq. (4.6) that we saw in Section 4.1

$$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30}f^{(5)}(\xi). \quad \square$$

Other formulas for first and higher derivatives can be derived in a similar manner. See, for example, Exercise 8.

The technique of extrapolation is used throughout the text. The most prominent applications occur in approximating integrals in Section 4.5 and for determining approximate solutions to differential equations in Section 5.8.

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## EXERCISE SET 4.2

**1.** Apply the extrapolation process described in Example 1 to determine $N_3(h)$, an approximation to $f'(x_0)$, for the following functions and stepsizes.

**a.** $f(x) = \ln x, x_0 = 1.0, h = 0.4$

**b.** $f(x) = x + e^x, x_0 = 0.0, h = 0.4$

**c.** $f(x) = 2^x \sin x, x_0 = 1.05, h = 0.4$

**d.** $f(x) = x^3 \cos x, x_0 = 2.3, h = 0.4$

**2.** Add another line to the extrapolation table in Exercise 1 to obtain the approximation $N_4(h)$.

**3.** Repeat Exercise 1 using four-digit rounding arithmetic.

**4.** Repeat Exercise 2 using four-digit rounding arithmetic.

**5.** The following data give approximations to the integral

$$M = \int_0^{\pi} \sin x \, dx.$$

$$N_1(h) = 1.570796, \quad N_1\left(\frac{h}{2}\right) = 1.896119, \quad N_1\left(\frac{h}{4}\right) = 1.974232, \quad N_1\left(\frac{h}{8}\right) = 1.993570.$$

Assuming $M = N_1(h) + K_1h^2 + K_2h^4 + K_3h^6 + K_4h^8 + O(h^{10})$, construct an extrapolation table to determine $N_4(h)$.

**6.** The following data can be used to approximate the integral

$$M = \int_0^{3\pi/2} \cos x \, dx.$$

$$N_1(h) = 2.356194, \qquad N_1\left(\frac{h}{2}\right) = -0.4879837,$$

$$N_1\left(\frac{h}{4}\right) = -0.8815732, \quad N_1\left(\frac{h}{8}\right) = -0.9709157.$$

Assume a formula exists of the type given in Exercise 5 and determine $N_4(h)$.

**7.** Show that the five-point formula in Eq. (4.6) applied to $f(x) = xe^x$ at $x_0 = 2.0$ gives $N_2(0.2)$ in Table 4.6 when $h = 0.1$ and $N_2(0.1)$ when $h = 0.05$.

**8.** The forward-difference formula can be expressed as

$$f'(x_0) = \frac{1}{h}[f(x_0 + h) - f(x_0)] - \frac{h}{2}f''(x_0) - \frac{h^2}{6}f'''(x_0) + O(h^3).$$

Use extrapolation to derive an $O(h^3)$ formula for $f'(x_0)$.

**9.** Suppose that $N(h)$ is an approximation to $M$ for every $h > 0$ and that

$$M = N(h) + K_1h + K_2h^2 + K_3h^3 + \cdots,$$

for some constants $K_1$, $K_2$, $K_3$, .... Use the values $N(h)$, $N\left(\frac{h}{3}\right)$, and $N\left(\frac{h}{9}\right)$ to produce an $O(h^3)$ approximation to $M$.

**10.** Suppose that $N(h)$ is an approximation to $M$ for every $h > 0$ and that

$$M = N(h) + K_1h^2 + K_2h^4 + K_3h^6 + \cdots,$$

for some constants $K_1$, $K_2$, $K_3$, .... Use the values $N(h)$, $N\left(\frac{h}{3}\right)$, and $N\left(\frac{h}{9}\right)$ to produce an $O(h^6)$ approximation to $M$.

**11.** In calculus, we learn that $e = \lim_{h\to 0}(1 + h)^{1/h}$.

**a.** Determine approximations to $e$ corresponding to $h = 0.04$, 0.02, and 0.01.

**b.** Use extrapolation on the approximations, assuming that constants $K_1$, $K_2$, ... exist with $e = (1 + h)^{1/h} + K_1h + K_2h^2 + K_3h^3 + \cdots$, to produce an $O(h^3)$ approximation to $e$, where $h = 0.04$.

**c.** Do you think that the assumption in part (b) is correct?

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**12.** **a.** Show that

$$\lim_{h\to 0}\left(\frac{2+h}{2-h}\right)^{1/h} = e.$$

**b.** Compute approximations to $e$ using the formula $N(h) = \left(\frac{2+h}{2-h}\right)^{1/h}$, for $h = 0.04$, $0.02$, and $0.01$.

**c.** Assume that $e = N(h) + K_1h + K_2h^2 + K_3h^3 + \cdots$. Use extrapolation, with at least 16 digits of precision, to compute an $O(h^3)$ approximation to $e$ with $h = 0.04$. Do you think the assumption is correct?

**d.** Show that $N(-h) = N(h)$.

**e.** Use part (d) to show that $K_1 = K_3 = K_5 = \cdots = 0$ in the formula

$$e = N(h) + K_1h + K_2h^2 + K_3h^3K_4h^4 + K_5h^5 + \cdots,$$

so that the formula reduces to

$$e = N(h) + K_2h^2 + K_4h^4 + K_6h^6 + \cdots.$$

**f.** Use the results of part (e) and extrapolation to compute an $O(h^6)$ approximation to $e$ with $h = 0.04$.

**13.** Suppose the following extrapolation table has been constructed to approximate the number $M$ with $M = N_1(h) + K_1h^2 + K_2h^4 + K_3h^6$:

| | | |
|---|---|---|
| $N_1(h)$ | | |
| $N_1\left(\frac{h}{2}\right)$ | $N_2(h)$ | |
| $N_1\left(\frac{h}{4}\right)$ | $N_2\left(\frac{h}{2}\right)$ | $N_3(h)$ |

**a.** Show that the linear interpolating polynomial $P_{0,1}(h)$ through $(h^2, N_1(h))$ and $(h^2/4, N_1(h/2))$ satisfies $P_{0,1}(0) = N_2(h)$. Similarly, show that $P_{1,2}(0) = N_2(h/2)$.

**b.** Show that the linear interpolating polynomial $P_{0,2}(h)$ through $(h^4, N_2(h))$ and $(h^4/16, N_2(h/2))$ satisfies $P_{0,2}(0) = N_3(h)$.

**14.** Suppose that $N_1(h)$ is a formula that produces $O(h)$ approximations to a number $M$ and that

$$M = N_1(h) + K_1h + K_2h^2 + \cdots,$$

for a collection of positive constants $K_1, K_2, \ldots$. Then $N_1(h)$, $N_1(h/2)$, $N_1(h/4)$, ... are all lower bounds for $M$. What can be said about the extrapolated approximations $N_2(h), N_3(h), \ldots$?

**15.** The semiperimeters of regular polygons with $k$ sides that inscribe and circumscribe the unit circle were used by Archimedes before 200 B.C.E. to approximate $\pi$, the circumference of a semicircle. Geometry can be used to show that the sequence of inscribed and circumscribed semiperimeters $\{p_k\}$ and $\{P_k\}$, respectively, satisfy

$$p_k = k\sin\left(\frac{\pi}{k}\right) \quad \text{and} \quad P_k = k\tan\left(\frac{\pi}{k}\right),$$

with $p_k < \pi < P_k$, whenever $k \geq 4$.

**a.** Show that $p_4 = 2\sqrt{2}$ and $P_4 = 4$.

**b.** Show that for $k \geq 4$, the sequences satisfy the recurrence relations

$$P_{2k} = \frac{2p_kP_k}{p_k + P_k} \quad \text{and} \quad p_{2k} = \sqrt{p_kP_{2k}}.$$

**c.** Approximate $\pi$ to within $10^{-4}$ by computing $p_k$ and $P_k$ until $P_k - p_k < 10^{-4}$.

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**d.** Use Taylor Series to show that

$$\pi = p_k + \frac{\pi^3}{3!}\left(\frac{1}{k}\right)^2 - \frac{\pi^5}{5!}\left(\frac{1}{k}\right)^4 + \cdots$$

and

$$\pi = P_k - \frac{\pi^3}{3}\left(\frac{1}{k}\right)^2 + \frac{2\pi^5}{15}\left(\frac{1}{k}\right)^4 - \cdots.$$

**e.** Use extrapolation with $h = 1/k$ to better approximate $\pi$.

## 4.3 Elements of Numerical Integration

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain. The basic method involved in approximating $\int_a^b f(x)\,dx$ is called **numerical quadrature**. It uses a sum $\sum_{i=0}^n a_i f(x_i)$ to approximate $\int_a^b f(x)\,dx$.

The methods of quadrature in this section are based on the interpolation polynomials given in Chapter 3. The basic idea is to select a set of distinct nodes $\{x_0, \ldots, x_n\}$ from the interval $[a, b]$. Then integrate the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$$

and its truncation error term over $[a, b]$ to obtain

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)\,dx + \int_a^b \prod_{i=0}^{n}(x - x_i)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,dx \\ &= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x - x_i) f^{(n+1)}(\xi(x))\,dx,\end{aligned}$$

where $\xi(x)$ is in $[a, b]$ for each $x$ and

$$a_i = \int_a^b L_i(x)\,dx, \quad \text{for each } i = 0, 1, \ldots, n.$$

The quadrature formula is, therefore,

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

with error given by

$$E(f) = \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x - x_i) f^{(n+1)}(\xi(x))\,dx.$$

Before discussing the general situation of quadrature formulas, let us consider formulas produced by using first and second Lagrange polynomials with equally-spaced nodes. This gives the **Trapezoidal rule** and **Simpson's rule**, which are commonly introduced in calculus courses.

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## The Trapezoidal Rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x)\,dx$, let $x_0 = a$, $x_1 = b$, $h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1).$$

Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \left[ \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx + \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx. \tag{4.23}$$

The product $(x - x_0)(x - x_1)$ does not change sign on $[x_0, x_1]$, so the Weighted Mean Value Theorem for Integrals 1.13 can be applied to the error term to give, for some $\xi$ in $(x_0, x_1)$,

$$\begin{aligned} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx &= f''(\xi) \int_{x_0}^{x_1} (x - x_0)(x - x_1)\,dx \\ &= f''(\xi) \left[ \frac{x^3}{3} - \frac{(x_1 + x_0)}{2} x^2 + x_0 x_1 x \right]_{x_0}^{x_1} \\ &= -\frac{h^3}{6} f''(\xi). \end{aligned}$$

When we use the term *trapezoid* we mean a four-sided figure that has at least two of its sides parallel. The European term for this figure is *trapezium*. To further confuse the issue, the European word trapezoidal refers to a four-sided figure with no sides equal, and the American word for this type of figure is trapezium.

Consequently, Eq. (4.23) implies that

$$\begin{aligned} \int_a^b f(x)\,dx &= \left[ \frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\xi) \\ &= \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi). \end{aligned}$$

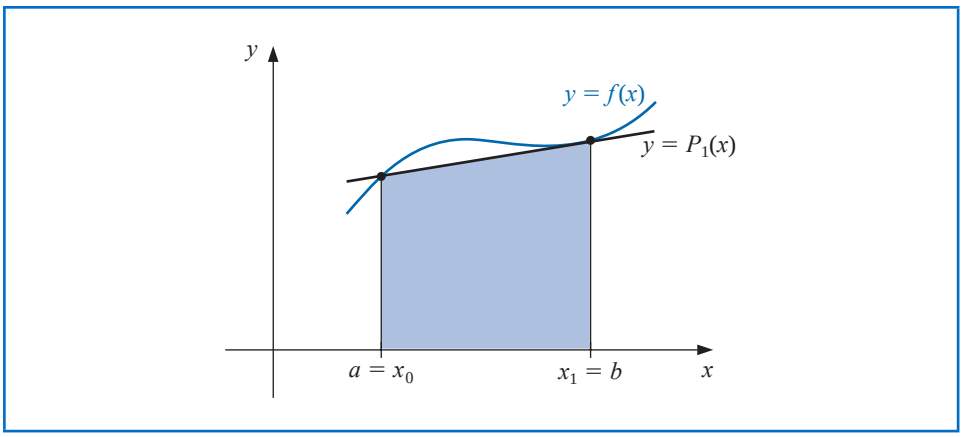
Using the notation $h = x_1 - x_0$ gives the following rule:

### Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).$$

This is called the Trapezoidal rule because when $f$ is a function with positive values, $\int_a^b f(x)\,dx$ is approximated by the area in a trapezoid, as shown in Figure 4.3.

**Figure 4.3**

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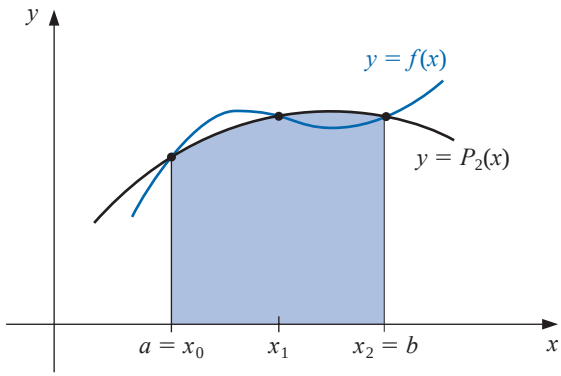
The error term for the Trapezoidal rule involves $f''$, so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is, any polynomial of degree one or less.

## Simpson's Rule

Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$. (See Figure 4.4.)

**Figure 4.4**




Therefore

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} \left[ \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx + \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x))\,dx.$$

Deriving Simpson's rule in this manner, however, provides only an $O(h^4)$ error term involving $f^{(3)}$. By approaching the problem in another way, a higher-order term involving $f^{(4)}$ can be derived.

To illustrate this alternative method, suppose that $f$ is expanded in the third Taylor polynomial about $x_1$. Then for each $x$ in $[x_0, x_2]$, a number $\xi(x)$ in $(x_0, x_2)$ exists with

$$f(x) = f(x_1) + f'(x_1)(x-x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4$$

and

$$\int_{x_0}^{x_2} f(x)\,dx = \left[ f(x_1)(x-x_1) + \frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f'''(x_1)}{24}(x-x_1)^4 \right]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx. \quad (4.24)$$

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Because $(x - x_1)^4$ is never negative on $[x_0, x_2]$, the Weighted Mean Value Theorem for Integrals 1.13 implies that

$$\frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x - x_1)^4\,dx = \frac{f^{(4)}(\xi_1)}{120}(x - x_1)^5\Big]_{x_0}^{x_2},$$

for some number $\xi_1$ in $(x_0, x_2)$.

However, $h = x_2 - x_1 = x_1 - x_0$, so

$$(x_2 - x_1)^2 - (x_0 - x_1)^2 = (x_2 - x_1)^4 - (x_0 - x_1)^4 = 0,$$

whereas

$$(x_2 - x_1)^3 - (x_0 - x_1)^3 = 2h^3 \quad \text{and} \quad (x_2 - x_1)^5 - (x_0 - x_1)^5 = 2h^5.$$

Consequently, Eq. (4.24) can be rewritten as

$$\int_{x_0}^{x_2} f(x)\,dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + \frac{f^{(4)}(\xi_1)}{60}h^5.$$

If we now replace $f''(x_1)$ by the approximation given in Eq. (4.9) of Section 4.1, we have

$$\begin{aligned}\int_{x_0}^{x_2} f(x)\,dx &= 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12}f^{(4)}(\xi_2)\right\} + \frac{f^{(4)}(\xi_1)}{60}h^5\\ &= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12}\left[\frac{1}{3}f^{(4)}(\xi_2) - \frac{1}{5}f^{(4)}(\xi_1)\right].\end{aligned}$$

It can be shown by alternative methods (see Exercise 24) that the values $\xi_1$ and $\xi_2$ in this expression can be replaced by a common value $\xi$ in $(x_0, x_2)$. This gives Simpson's rule.

Thomas Simpson (1710–1761) was a self-taught mathematician who supported himself during his early years as a weaver. His primary interest was probability theory, although in 1750 he published a two-volume calculus book entitled *The Doctrine and Application of Fluxions*.

### Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi).$$

The error term in Simpson's rule involves the fourth derivative of $f$, so it gives exact results when applied to any polynomial of degree three or less.

**Example 1** Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)\,dx$ when $f(x)$ is

**(a)** $x^2$ **(b)** $x^4$ **(c)** $(x+1)^{-1}$
**(d)** $\sqrt{1+x^2}$ **(e)** $\sin x$ **(f)** $e^x$

***Solution*** On $[0, 2]$ the Trapezoidal and Simpson's rule have the forms

$$\text{Trapezoid:} \quad \int_0^2 f(x)\,dx \approx f(0) + f(2) \quad \text{and}$$

$$\text{Simpson's:} \quad \int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

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When $f(x) = x^2$ they give

$$\text{Trapezoid: } \int_0^2 f(x)\,dx \approx 0^2 + 2^2 = 4 \quad \text{and}$$

$$\text{Simpson's: } \int_0^2 f(x)\,dx \approx \frac{1}{3}[(0^2) + 4 \cdot 1^2 + 2^2] = \frac{8}{3}.$$

The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.

The results to three places for the functions are summarized in Table 4.7. Notice that in each instance Simpson's Rule is significantly superior. ■

**Table 4.7**

| | (a) | (b) | (c) | (d) | (e) | (f) |
|---|---|---|---|---|---|---|
| $f(x)$ | $x^2$ | $x^4$ | $(x+1)^{-1}$ | $\sqrt{1+x^2}$ | $\sin x$ | $e^x$ |
| Exact value | 2.667 | 6.400 | 1.099 | 2.958 | 1.416 | 6.389 |
| Trapezoidal | 4.000 | 16.000 | 1.333 | 3.326 | 0.909 | 8.389 |
| Simpson's | 2.667 | 6.667 | 1.111 | 2.964 | 1.425 | 6.421 |

## Measuring Precision

The standard derivation of quadrature error formulas is based on determining the class of polynomials for which these formulas produce exact results. The next definition is used to facilitate the discussion of this derivation.

***Definition 4.1*** The **degree of accuracy**, or **precision**, of a quadrature formula is the largest positive integer $n$ such that the formula is exact for $x^k$, for each $k = 0, 1, \ldots, n$. ■

The improved accuracy of Simpson's rule over the Trapezoidal rule is intuitively explained by the fact that Simpson's rule includes a midpoint evaluation that provides better balance to the approximation.

Definition 4.1 implies that the Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.

Integration and summation are linear operations; that is,

$$\int_a^b (\alpha f(x) + \beta g(x))\,dx = \alpha \int_a^b f(x)\,dx + \beta \int_a^b g(x)\,dx$$

and

$$\sum_{i=0}^{n} (\alpha f(x_i) + \beta g(x_i)) = \alpha \sum_{i=0}^{n} f(x_i) + \beta \sum_{i=0}^{n} g(x_i),$$

for each pair of integrable functions $f$ and $g$ and each pair of real constants $\alpha$ and $\beta$. This implies (see Exercise 25) that:

The open and closed terminology for methods implies that the open methods use as nodes only points in the open interval, $(a, b)$ to approximate $\int_a^b f(x)\,dx$. The closed methods include the points $a$ and $b$ of the closed interval $[a, b]$ as nodes.

- The degree of precision of a quadrature formula is $n$ if and only if the error is zero for all polynomials of degree $k = 0, 1, \ldots, n$, but is not zero for some polynomial of degree $n + 1$.

The Trapezoidal and Simpson's rules are examples of a class of methods known as Newton-Cotes formulas. There are two types of Newton-Cotes formulas, open and closed.

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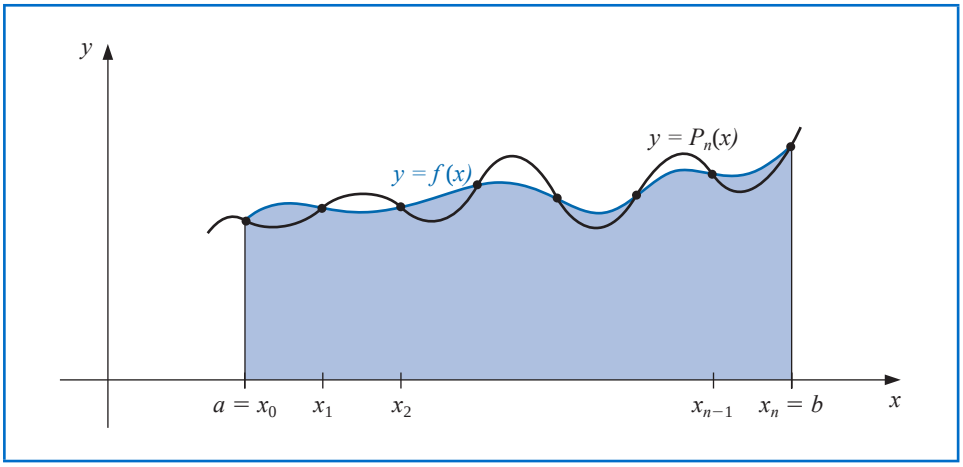
## Closed Newton-Cotes Formulas

The $(n+1)$-*point closed Newton-Cotes formula* uses nodes $x_i = x_0 + ih$, for $i = 0, 1, \ldots, n$, where $x_0 = a$, $x_n = b$ and $h = (b-a)/n$. (See Figure 4.5.) It is called closed because the endpoints of the closed interval $[a, b]$ are included as nodes.

**Figure 4.5**




The formula assumes the form

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

where

$$a_i = \int_{x_0}^{x_n} L_i(x)\,dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}\,dx.$$

The following theorem details the error analysis associated with the closed Newton-Cotes formulas. For a proof of this theorem, see [IK], p. 313.

**Theorem 4.2** Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes formula with $x_0 = a$, $x_n = b$, and $h = (b-a)/n$. There exists $\xi \in (a, b)$ for which

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)\,dt,$$

if $n$ is even and $f \in C^{n+2}[a, b]$, and

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)\,dt,$$

if $n$ is odd and $f \in C^{n+1}[a, b]$. ■

Roger Cotes (1682–1716) rose from a modest background to become, in 1704, the first Plumian Professor at Cambridge University. He made advances in numerous mathematical areas including numerical methods for interpolation and integration. Newton is reputed to have said of Cotes ...*if he had lived we might have known something.*

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Note that when $n$ is an even integer, the degree of precision is $n + 1$, although the interpolation polynomial is of degree at most $n$. When $n$ is odd, the degree of precision is only $n$.

Some of the common **closed Newton-Cotes formulas** with their error terms are listed. Note that in each case the unknown value $\xi$ lies in $(a, b)$.

### $n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi), \quad \text{where} \quad x_0 < \xi < x_1. \tag{4.25}$$

### $n = 2$: Simpson's rule

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi), \quad \text{where} \quad x_0 < \xi < x_2. \tag{4.26}$$

### $n = 3$: Simpson's Three-Eighths rule

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi), \tag{4.27}$$

$$\text{where} \quad x_0 < \xi < x_3.$$

### $n = 4$:

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] - \frac{8h^7}{945} f^{(6)}(\xi),$$

$$\text{where} \quad x_0 < \xi < x_4. \tag{4.28}$$

## Open Newton-Cotes Formulas

The *open Newton-Cotes formulas* do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, for each $i = 0, 1, \ldots, n$, where $h = (b - a)/(n + 2)$ and $x_0 = a + h$. This implies that $x_n = b - h$, so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$, as shown in Figure 4.6 on page 200. Open formulas contain all the nodes used for the approximation within the open interval $(a, b)$. The formulas become

$$\int_a^b f(x)\,dx = \int_{x_{-1}}^{x_{n+1}} f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

where

$$a_i = \int_a^b L_i(x)\,dx.$$

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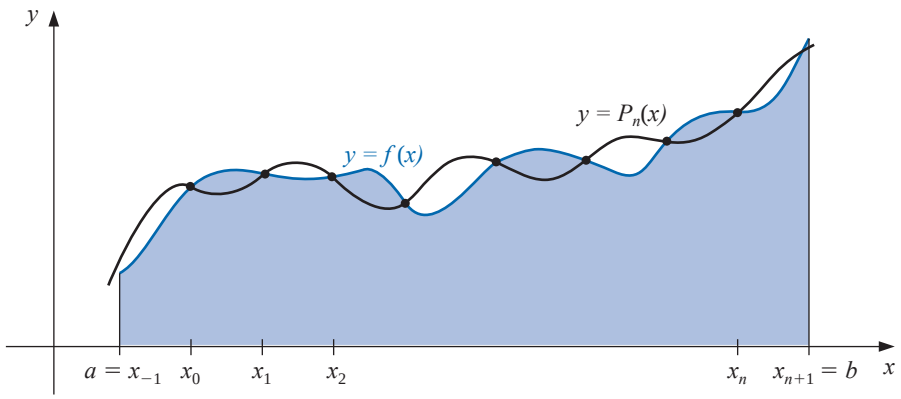
**Figure 4.6**




The following theorem is analogous to Theorem 4.2; its proof is contained in [IK], p. 314.

***Theorem 4.3*** Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point open Newton-Cotes formula with $x_{-1} = a$, $x_{n+1} = b$, and $h = (b-a)/(n+2)$. There exists $\xi \in (a, b)$ for which

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt,$$

if $n$ is even and $f \in C^{n+2}[a, b]$, and

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt,$$

if $n$ is odd and $f \in C^{n+1}[a, b]$. ■

Notice, as in the case of the closed methods, we have the degree of precision comparatively higher for the even methods than for the odd methods.

Some of the common **open Newton-Cotes** formulas with their error terms are as follows:

### $n = 0$: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_1. \tag{4.29}$$

### $n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4} f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_2. \tag{4.30}$$

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### $n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45}f^{(4)}(\xi), \tag{4.31}$$

where $x_{-1} < \xi < x_3$.

### $n = 3$:

$$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95}{144}h^5 f^{(4)}(\xi), \tag{4.32}$$

where $x_{-1} < \xi < x_4$.

**Example 2** Compare the results of the closed and open Newton-Cotes formulas listed as (4.25)–(4.28) and (4.29)–(4.32) when approximating

$$\int_0^{\pi/4} \sin x\,dx = 1 - \sqrt{2}/2 \approx 0.29289322.$$

***Solution*** For the closed formulas we have

$$n = 1: \quad \frac{(\pi/4)}{2}\left[\sin 0 + \sin\frac{\pi}{4}\right] \approx 0.27768018$$

$$n = 2: \quad \frac{(\pi/8)}{3}\left[\sin 0 + 4\sin\frac{\pi}{8} + \sin\frac{\pi}{4}\right] \approx 0.29293264$$

$$n = 3: \quad \frac{3(\pi/12)}{8}\left[\sin 0 + 3\sin\frac{\pi}{12} + 3\sin\frac{\pi}{6} + \sin\frac{\pi}{4}\right] \approx 0.29291070$$

$$n = 4: \quad \frac{2(\pi/16)}{45}\left[7\sin 0 + 32\sin\frac{\pi}{16} + 12\sin\frac{\pi}{8} + 32\sin\frac{3\pi}{16} + 7\sin\frac{\pi}{4}\right] \approx 0.29289318$$

and for the open formulas we have

$$n = 0: \quad 2(\pi/8)\left[\sin\frac{\pi}{8}\right] \approx 0.30055887$$

$$n = 1: \quad \frac{3(\pi/12)}{2}\left[\sin\frac{\pi}{12} + \sin\frac{\pi}{6}\right] \approx 0.29798754$$

$$n = 2: \quad \frac{4(\pi/16)}{3}\left[2\sin\frac{\pi}{16} - \sin\frac{\pi}{8} + 2\sin\frac{3\pi}{16}\right] \approx 0.29285866$$

$$n = 3: \quad \frac{5(\pi/20)}{24}\left[11\sin\frac{\pi}{20} + \sin\frac{\pi}{10} + \sin\frac{3\pi}{20} + 11\sin\frac{\pi}{5}\right] \approx 0.29286923$$

Table 4.8 summarizes these results and shows the approximation errors. ■

**Table 4.8**

| $n$ | 0 | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| Closed formulas | | 0.27768018 | 0.29293264 | 0.29291070 | 0.29289318 |
| Error | | 0.01521303 | 0.00003942 | 0.00001748 | 0.00000004 |
| Open formulas | 0.30055887 | 0.29798754 | 0.29285866 | 0.29286923 | |
| Error | 0.00766565 | 0.00509432 | 0.00003456 | 0.00002399 | |

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## EXERCISE SET 4.3

**1.** Approximate the following integrals using the Trapezoidal rule.

**a.** $\int_{0.5}^{1} x^4\,dx$ **b.** $\int_{0}^{0.5} \frac{2}{x-4}\,dx$

**c.** $\int_{1}^{1.5} x^2 \ln x\,dx$ **d.** $\int_{0}^{1} x^2 e^{-x}\,dx$

**e.** $\int_{1}^{1.6} \frac{2x}{x^2-4}\,dx$ **f.** $\int_{0}^{0.35} \frac{2}{x^2-4}\,dx$

**g.** $\int_{0}^{\pi/4} x \sin x\,dx$ **h.** $\int_{0}^{\pi/4} e^{3x} \sin 2x\,dx$

**2.** Approximate the following integrals using the Trapezoidal rule.

**a.** $\int_{-0.25}^{0.25} (\cos x)^2\,dx$ **b.** $\int_{-0.5}^{0} x \ln(x+1)\,dx$

**c.** $\int_{0.75}^{1.3} \left((\sin x)^2 - 2x \sin x + 1\right)\,dx$ **d.** $\int_{e}^{e+1} \frac{1}{x \ln x}\,dx$

**3.** Find a bound for the error in Exercise 1 using the error formula, and compare this to the actual error.

**4.** Find a bound for the error in Exercise 2 using the error formula, and compare this to the actual error.

**5.** Repeat Exercise 1 using Simpson's rule.

**6.** Repeat Exercise 2 using Simpson's rule.

**7.** Repeat Exercise 3 using Simpson's rule and the results of Exercise 5.

**8.** Repeat Exercise 4 using Simpson's rule and the results of Exercise 6.

**9.** Repeat Exercise 1 using the Midpoint rule.

**10.** Repeat Exercise 2 using the Midpoint rule.

**11.** Repeat Exercise 3 using the Midpoint rule and the results of Exercise 9.

**12.** Repeat Exercise 4 using the Midpoint rule and the results of Exercise 10.

**13.** The Trapezoidal rule applied to $\int_0^2 f(x)\,dx$ gives the value 4, and Simpson's rule gives the value 2. What is $f(1)$?

**14.** The Trapezoidal rule applied to $\int_0^2 f(x)\,dx$ gives the value 5, and the Midpoint rule gives the value 4. What value does Simpson's rule give?

**15.** Find the degree of precision of the quadrature formula

$$\int_{-1}^{1} f(x)\,dx = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).$$

**16.** Let $h = (b-a)/3$, $x_0 = a$, $x_1 = a+h$, and $x_2 = b$. Find the degree of precision of the quadrature formula

$$\int_a^b f(x)\,dx = \frac{9}{4}hf(x_1) + \frac{3}{4}hf(x_2).$$

**17.** The quadrature formula $\int_{-1}^{1} f(x)\,dx = c_0 f(-1) + c_1 f(0) + c_2 f(1)$ is exact for all polynomials of degree less than or equal to 2. Determine $c_0$, $c_1$, and $c_2$.

**18.** The quadrature formula $\int_0^2 f(x)\,dx = c_0 f(0) + c_1 f(1) + c_2 f(2)$ is exact for all polynomials of degree less than or equal to 2. Determine $c_0$, $c_1$, and $c_2$.

**19.** Find the constants $c_0$, $c_1$, and $x_1$ so that the quadrature formula

$$\int_0^1 f(x)\,dx = c_0 f(0) + c_1 f(x_1)$$

has the highest possible degree of precision.

**20.** Find the constants $x_0$, $x_1$, and $c_1$ so that the quadrature formula

$$\int_0^1 f(x)\,dx = \frac{1}{2} f(x_0) + c_1 f(x_1)$$

has the highest possible degree of precision.

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**21.** Approximate the following integrals using formulas (4.25) through (4.32). Are the accuracies of the approximations consistent with the error formulas? Which of parts (d) and (e) give the better approximation?

**a.** $\int_0^{0.1} \sqrt{1+x}\,dx$ **b.** $\int_0^{\pi/2} (\sin x)^2\,dx$

**c.** $\int_{1.1}^{1.5} e^x\,dx$ **d.** $\int_1^{10} \frac{1}{x}\,dx$

**e.** $\int_1^{5.5} \frac{1}{x}\,dx + \int_{5.5}^{10} \frac{1}{x}\,dx$ **f.** $\int_0^1 x^{1/3}\,dx$

**22.** Given the function $f$ at the following values,

| $x$ | 1.8 | 2.0 | 2.2 | 2.4 | 2.6 |
|---|---|---|---|---|---|
| $f(x)$ | 3.12014 | 4.42569 | 6.04241 | 8.03014 | 10.46675 |

approximate $\int_{1.8}^{2.6} f(x)\,dx$ using all the appropriate quadrature formulas of this section.

**23.** Suppose that the data of Exercise 22 have round-off errors given by the following table.

| $x$ | 1.8 | 2.0 | 2.2 | 2.4 | 2.6 |
|---|---|---|---|---|---|
| Error in $f(x)$ | $2 \times 10^{-6}$ | $-2 \times 10^{-6}$ | $-0.9 \times 10^{-6}$ | $-0.9 \times 10^{-6}$ | $2 \times 10^{-6}$ |

Calculate the errors due to round-off in Exercise 22.

**24.** Derive Simpson's rule with error term by using

$$\int_{x_0}^{x_2} f(x)\,dx = a_0 f(x_0) + a_1 f(x_1) + a_2 f(x_2) + k f^{(4)}(\xi).$$

Find $a_0, a_1$, and $a_2$ from the fact that Simpson's rule is exact for $f(x) = x^n$ when $n = 1, 2$, and 3. Then find $k$ by applying the integration formula with $f(x) = x^4$.

**25.** Prove the statement following Definition 4.1; that is, show that a quadrature formula has degree of precision $n$ if and only if the error $E(P(x)) = 0$ for all polynomials $P(x)$ of degree $k = 0, 1, \ldots, n$, but $E(P(x)) \neq 0$ for some polynomial $P(x)$ of degree $n + 1$.

**26.** Derive Simpson's three-eighths rule (the closed rule with $n = 3$) with error term by using Theorem 4.2.

**27.** Derive the open rule with $n = 1$ with error term by using Theorem 4.3.

## 4.4 Composite Numerical Integration

The Newton-Cotes formulas are generally unsuitable for use over large integration intervals. High-degree formulas would be required, and the values of the coefficients in these formulas are difficult to obtain. Also, the Newton-Cotes formulas are based on interpolatory polynomials that use equally-spaced nodes, a procedure that is inaccurate over large intervals because of the oscillatory nature of high-degree polynomials.

Piecewise approximation is often effective. Recall that this was used for spline interpolation.

In this section, we discuss a *piecewise* approach to numerical integration that uses the low-order Newton-Cotes formulas. These are the techniques most often applied.

**Example 1** Use Simpson's rule to approximate $\int_0^4 e^x\,dx$ and compare this to the results obtained by adding the Simpson's rule approximations for $\int_0^2 e^x\,dx$ and $\int_2^4 e^x\,dx$. Compare these approximations to the sum of Simpson's rule for $\int_0^1 e^x\,dx$, $\int_1^2 e^x\,dx$, $\int_2^3 e^x\,dx$, and $\int_3^4 e^x\,dx$.

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***Solution*** Simpson's rule on $[0, 4]$ uses $h = 2$ and gives

$$\int_0^4 e^x\,dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958.$$

The exact answer in this case is $e^4 - e^0 = 53.59815$, and the error $-3.17143$ is far larger than we would normally accept.

Applying Simpson's rule on each of the intervals $[0, 2]$ and $[2, 4]$ uses $h = 1$ and gives

$$\begin{aligned}\int_0^4 e^x\,dx &= \int_0^2 e^x\,dx + \int_2^4 e^x\,dx\\ &\approx \frac{1}{3}\left(e^0 + 4e + e^2\right) + \frac{1}{3}\left(e^2 + 4e^3 + e^4\right)\\ &= \frac{1}{3}\left(e^0 + 4e + 2e^2 + 4e^3 + e^4\right)\\ &= 53.86385.\end{aligned}$$

The error has been reduced to $-0.26570$.

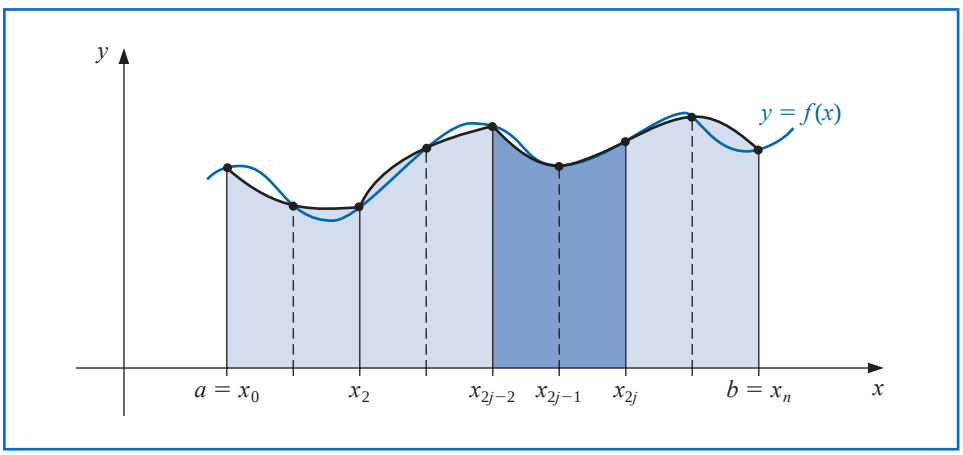
For the integrals on $[0, 1]$,$[1, 2]$,$[3, 4]$, and $[3, 4]$ we use Simpson's rule four times with $h = \frac{1}{2}$ giving

$$\begin{aligned}\int_0^4 e^x\,dx &= \int_0^1 e^x\,dx + \int_1^2 e^x\,dx + \int_2^3 e^x\,dx + \int_3^4 e^x\,dx\\ &\approx \frac{1}{6}\left(e_0 + 4e^{1/2} + e\right) + \frac{1}{6}\left(e + 4e^{3/2} + e^2\right)\\ &\quad + \frac{1}{6}\left(e^2 + 4e^{5/2} + e^3\right) + \frac{1}{6}\left(e^3 + 4e^{7/2} + e^4\right)\\ &= \frac{1}{6}\left(e^0 + 4e^{1/2} + 2e + 4e^{3/2} + 2e^2 + 4e^{5/2} + 2e^3 + 4e^{7/2} + e^4\right)\\ &= 53.61622.\end{aligned}$$

The error for this approximation has been reduced to $-0.01807$. ■

To generalize this procedure for an arbitrary integral $\int_a^b f(x)\,dx$, choose an even integer $n$. Subdivide the interval $[a, b]$ into $n$ subintervals, and apply Simpson's rule on each consecutive pair of subintervals. (See Figure 4.7.)

**Figure 4.7**

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With $h = (b-a)/n$ and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$, we have

$$\int_a^b f(x)\,dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx$$

$$= \sum_{j=1}^{n/2} \left\{ \frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\},$$

for some $\xi_j$ with $x_{2j-2} < \xi_j < x_{2j}$, provided that $f \in C^4[a,b]$. Using the fact that for each $j = 1, 2, \ldots, (n/2) - 1$ we have $f(x_{2j})$ appearing in the term corresponding to the interval $[x_{2j-2}, x_{2j}]$ and also in the term corresponding to the interval $[x_{2j}, x_{2j+2}]$, we can reduce this sum to

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[ f(x_0) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] - \frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

The error associated with this approximation is

$$E(f) = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j),$$

where $x_{2j-2} < \xi_j < x_{2j}$, for each $j = 1, 2, \ldots, n/2$.

If $f \in C^4[a,b]$, the Extreme Value Theorem 1.9 implies that $f^{(4)}$ assumes its maximum and minimum in $[a,b]$. Since

$$\min_{x\in[a,b]} f^{(4)}(x) \le f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x),$$

we have

$$\frac{n}{2}\min_{x\in[a,b]} f^{(4)}(x) \le \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \frac{n}{2}\max_{x\in[a,b]} f^{(4)}(x)$$

and

$$\min_{x\in[a,b]} f^{(4)}(x) \le \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x).$$

By the Intermediate Value Theorem 1.11, there is a $\mu \in (a,b)$ such that

$$f^{(4)}(\mu) = \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

Thus

$$E(f) = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu),$$

or, since $h = (b-a)/n$,

$$E(f) = -\frac{(b-a)}{180} h^4 f^{(4)}(\mu).$$

These observations produce the following result.

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**Theorem 4.4** Let $f \in C^4[a, b]$, $n$ be even, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a, b)$ for which the **Composite Simpson's rule** for $n$ subintervals can be written with its error term as

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180}h^4 f^{(4)}(\mu).$$

■

Notice that the error term for the Composite Simpson's rule is $O(h^4)$, whereas it was $O(h^5)$ for the standard Simpson's rule. However, these rates are not comparable because for standard Simpson's rule we have $h$ fixed at $h = (b - a)/2$, but for Composite Simpson's rule we have $h = (b - a)/n$, for $n$ an even integer. This permits us to considerably reduce the value of $h$ when the Composite Simpson's rule is used.

Algorithm 4.1 uses the Composite Simpson's rule on $n$ subintervals. This is the most frequently used general-purpose quadrature algorithm.

ALGORITHM
**4.1**

## Composite Simpson's Rule

To approximate the integral $I = \int_a^b f(x)\,dx$:

INPUT endpoints $a, b$; even positive integer $n$.

OUTPUT approximation $XI$ to $I$.

*Step 1* Set $h = (b - a)/n$.

*Step 2* Set $XI0 = f(a) + f(b)$;
$XI1 = 0$; (*Summation of* $f(x_{2i-1})$.)
$XI2 = 0$. (*Summation of* $f(x_{2i})$.)

*Step 3* For $i = 1, \ldots, n - 1$ do Steps 4 and 5.

*Step 4* Set $X = a + ih$.

*Step 5* If $i$ is even then set $XI2 = XI2 + f(X)$
else set $XI1 = XI1 + f(X)$.

*Step 6* Set $XI = h(XI0 + 2 \cdot XI2 + 4 \cdot XI1)/3$.

*Step 7* OUTPUT ($XI$);
STOP.

■

The subdivision approach can be applied to any of the Newton-Cotes formulas. The extensions of the Trapezoidal (see Figure 4.8) and Midpoint rules are given without proof. The Trapezoidal rule requires only one interval for each application, so the integer $n$ can be either odd or even.

**Theorem 4.5** Let $f \in C^2[a, b]$, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a, b)$ for which the **Composite Trapezoidal rule** for $n$ subintervals can be written with its error term as

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu).$$

■

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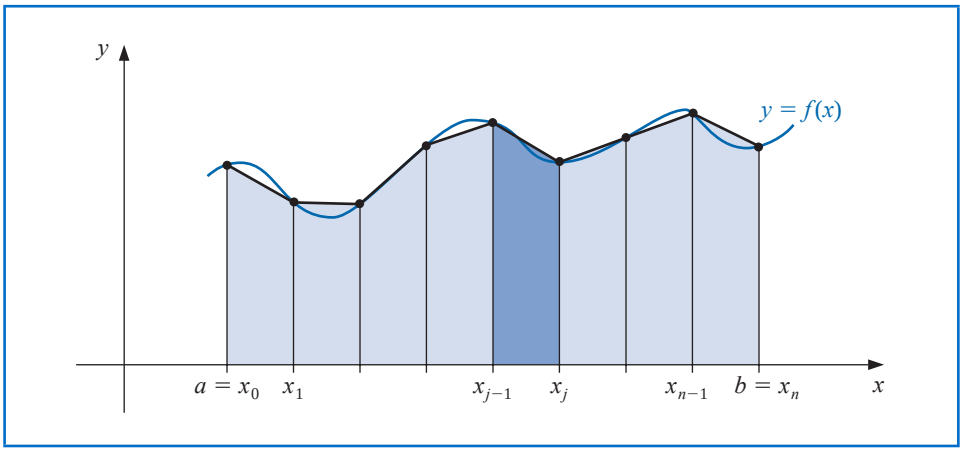
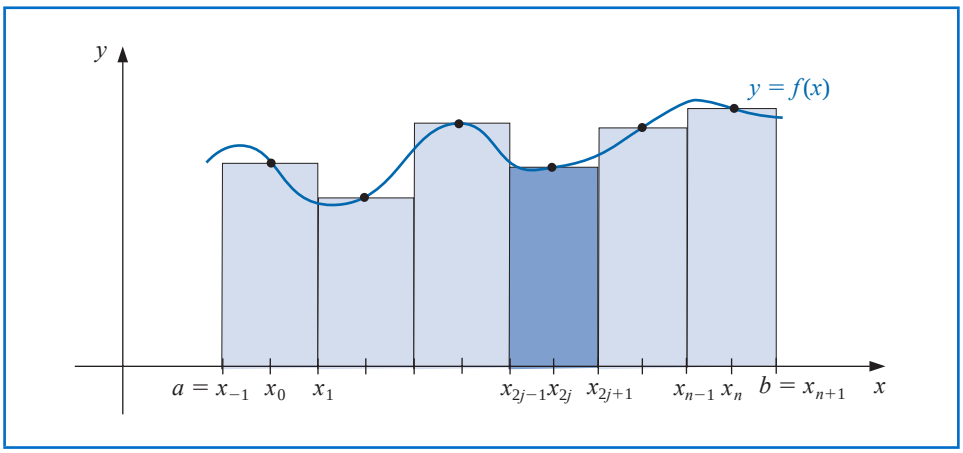
**Figure 4.8**




For the Composite Midpoint rule, $n$ must again be even. (See Figure 4.9.)

**Figure 4.9**




***Theorem 4.6*** Let $f \in C^2[a,b]$, $n$ be even, $h = (b-a)/(n+2)$, and $x_j = a + (j+1)h$ for each $j = -1, 0, \ldots, n+1$. There exists a $\mu \in (a,b)$ for which the **Composite Midpoint rule** for $n+2$ subintervals can be written with its error term as

$$\int_a^b f(x)\,dx = 2h\sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6}h^2 f''(\mu).$$

■

***Example 2*** Determine values of $h$ that will ensure an approximation error of less than 0.00002 when approximating $\int_0^{\pi} \sin x\,dx$ and employing
**(a)** Composite Trapezoidal rule and **(b)** Composite Simpson's rule.

***Solution*** **(a)** The error form for the Composite Trapezoidal rule for $f(x) = \sin x$ on $[0, \pi]$ is

$$\left|\frac{\pi h^2}{12} f''(\mu)\right| = \left|\frac{\pi h^2}{12}(-\sin\mu)\right| = \frac{\pi h^2}{12}|\sin\mu|.$$

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To ensure sufficient accuracy with this technique we need to have

$$\frac{\pi h^2}{12}|\sin\mu| \le \frac{\pi h^2}{12} < 0.00002.$$

Since $h = \pi/n$ implies that $n = \pi/h$, we need

$$\frac{\pi^3}{12n^2} < 0.00002 \quad \text{which implies that} \quad n > \left(\frac{\pi^3}{12(0.00002)}\right)^{1/2} \approx 359.44.$$

and the Composite Trapezoidal rule requires $n \ge 360$.

**(b)** The error form for the Composite Simpson's rule for $f(x) = \sin x$ on $[0, \pi]$ is

$$\left|\frac{\pi h^4}{180} f^{(4)}(\mu)\right| = \left|\frac{\pi h^4}{180}\sin\mu\right| = \frac{\pi h^4}{180}|\sin\mu|.$$

To ensure sufficient accuracy with this technique we need to have

$$\frac{\pi h^4}{180}|\sin\mu| \le \frac{\pi h^4}{180} < 0.00002.$$

Using again the fact that $n = \pi/h$ gives

$$\frac{\pi^5}{180n^4} < 0.00002 \quad \text{which implies that} \quad n > \left(\frac{\pi^5}{180(0.00002)}\right)^{1/4} \approx 17.07.$$

So Composite Simpson's rule requires only $n \ge 18$.

Composite Simpson's rule with $n = 18$ gives

$$\int_0^\pi \sin x\,dx \approx \frac{\pi}{54}\left[2\sum_{j=1}^{8}\sin\left(\frac{j\pi}{9}\right) + 4\sum_{j=1}^{9}\sin\left(\frac{(2j-1)\pi}{18}\right)\right] = 2.0000104.$$

This is accurate to within about $10^{-5}$ because the true value is $-\cos(\pi) - (-\cos(0)) = 2$. ■

Composite Simpson's rule is the clear choice if you wish to minimize computation. For comparison purposes, consider the Composite Trapezoidal rule using $h = \pi/18$ for the integral in Example 2. This approximation uses the same function evaluations as Composite Simpson's rule but the approximation in this case

$$\int_0^\pi \sin x\,dx \approx \frac{\pi}{36}\left[2\sum_{j=1}^{17}\sin\left(\frac{j\pi}{18}\right) + \sin 0 + \sin\pi\right] = \frac{\pi}{36}\left[2\sum_{j=1}^{17}\sin\left(\frac{j\pi}{18}\right)\right] = 1.9949205.$$

is accurate only to about $5 \times 10^{-3}$.

Maple contains numerous procedures for numerical integration in the *NumericalAnalysis* subpackage of the *Student* package. First access the library as usual with

*with*(*Student*[*NumericalAnalysis*])

The command for all methods is *Quadrature* with the options in the call specifying the method to be used. We will use the Trapezoidal method to illustrate the procedure. First define the function and the interval of integration with

$f := x \to \sin(x)$; $a := 0.0$; $b := \pi$

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After Maple responds with the function and the interval, enter the command

$$Quadrature(f(x), x = a..b, method = trapezoid, partition = 20, output = value)$$

$$1.995885973$$

The value of the step size $h$ in this instance is the width of the interval $b - a$ divided by the number specified by $partition = 20$.

Simpson's method can be called in a similar manner, except that the step size $h$ is determined by $b - a$ divided by twice the value of *partition*. Hence, the Simpson's rule approximation using the same nodes as those in the Trapezoidal rule is called with

$$Quadrature(f(x), x = a..b, method = simpson, partition = 10, output = value)$$

$$2.000006785$$

Any of the Newton-Cotes methods can be called using the option

$$method = newtoncotes[open, n] \quad \text{or} \quad method = newtoncotes[closed, n]$$

Be careful to correctly specify the number in *partition* when an even number of divisions is required, and when an open method is employed.

## Round-Off Error Stability

In Example 2 we saw that ensuring an accuracy of $2 \times 10^{-5}$ for approximating $\int_0^{\pi} \sin x\, dx$ required 360 subdivisions of $[0, \pi]$ for the Composite Trapezoidal rule and only 18 for Composite Simpson's rule. In addition to the fact that less computation is needed for the Simpson's technique, you might suspect that because of fewer computations this method would also involve less round-off error. However, an important property shared by all the composite integration techniques is a stability with respect to round-off error. That is, the round-off error does not depend on the number of calculations performed.

Numerical integration is expected to be stable, whereas numerical differentiation is unstable.

To demonstrate this rather amazing fact, suppose we apply the Composite Simpson's rule with $n$ subintervals to a function $f$ on $[a, b]$ and determine the maximum bound for the round-off error. Assume that $f(x_i)$ is approximated by $\tilde{f}(x_i)$ and that

$$f(x_i) = \tilde{f}(x_i) + e_i, \quad \text{for each } i = 0, 1, \ldots, n,$$

where $e_i$ denotes the round-off error associated with using $\tilde{f}(x_i)$ to approximate $f(x_i)$. Then the accumulated error, $e(h)$, in the Composite Simpson's rule is

$$\begin{aligned} e(h) &= \left| \frac{h}{3} \left[ e_0 + 2 \sum_{j=1}^{(n/2)-1} e_{2j} + 4 \sum_{j=1}^{n/2} e_{2j-1} + e_n \right] \right| \\ &\leq \frac{h}{3} \left[ |e_0| + 2 \sum_{j=1}^{(n/2)-1} |e_{2j}| + 4 \sum_{j=1}^{n/2} |e_{2j-1}| + |e_n| \right]. \end{aligned}$$

If the round-off errors are uniformly bounded by $\varepsilon$, then

$$e(h) \leq \frac{h}{3} \left[ \varepsilon + 2 \left( \frac{n}{2} - 1 \right) \varepsilon + 4 \left( \frac{n}{2} \right) \varepsilon + \varepsilon \right] = \frac{h}{3} 3n\varepsilon = nh\varepsilon.$$

But $nh = b - a$, so

$$e(h) \leq (b - a)\varepsilon,$$

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a bound independent of $h$ (and $n$). This means that, even though we may need to divide an interval into more parts to ensure accuracy, the increased computation that is required does not increase the round-off error. This result implies that the procedure is stable as $h$ approaches zero. Recall that this was not true of the numerical differentiation procedures considered at the beginning of this chapter.

## EXERCISE SET 4.4

**1.** Use the Composite Trapezoidal rule with the indicated values of $n$ to approximate the following integrals.

**a.** $\int_1^2 x \ln x \, dx, \quad n = 4$

**b.** $\int_{-2}^2 x^3 e^x \, dx, \quad n = 4$

**c.** $\int_0^2 \frac{2}{x^2 + 4} \, dx, \quad n = 6$

**d.** $\int_0^{\pi} x^2 \cos x \, dx, \quad n = 6$

**e.** $\int_0^2 e^{2x} \sin 3x \, dx, \quad n = 8$

**f.** $\int_1^3 \frac{x}{x^2 + 4} \, dx, \quad n = 8$

**g.** $\int_3^5 \frac{1}{\sqrt{x^2 - 4}} \, dx, \quad n = 8$

**h.** $\int_0^{3\pi/8} \tan x \, dx, \quad n = 8$

**2.** Use the Composite Trapezoidal rule with the indicated values of $n$ to approximate the following integrals.

**a.** $\int_{-0.5}^{0.5} \cos^2 x \, dx, \quad n = 4$

**b.** $\int_{-0.5}^{0.5} x \ln(x + 1) \, dx, \quad n = 6$

**c.** $\int_{.75}^{1.75} (\sin^2 x - 2x \sin x + 1) \, dx, \quad n = 8$

**d.** $\int_e^{e+2} \frac{1}{x \ln x} \, dx, \quad n = 8$

**3.** Use the Composite Simpson's rule to approximate the integrals in Exercise 1.

**4.** Use the Composite Simpson's rule to approximate the integrals in Exercise 2.

**5.** Use the Composite Midpoint rule with $n + 2$ subintervals to approximate the integrals in Exercise 1.

**6.** Use the Composite Midpoint rule with $n + 2$ subintervals to approximate the integrals in Exercise 2.

**7.** Approximate $\int_0^2 x^2 \ln(x^2 + 1) \, dx$ using $h = 0.25$. Use

**a.** Composite Trapezoidal rule.

**b.** Composite Simpson's rule.

**c.** Composite Midpoint rule.

**8.** Approximate $\int_0^2 x^2 e^{-x^2} \, dx$ using $h = 0.25$. Use

**a.** Composite Trapezoidal rule.

**b.** Composite Simpson's rule.

**c.** Composite Midpoint rule.

**9.** Suppose that $f(0) = 1$, $f(0.5) = 2.5$, $f(1) = 2$, and $f(0.25) = f(0.75) = \alpha$. Find $\alpha$ if the Composite Trapezoidal rule with $n = 4$ gives the value 1.75 for $\int_0^1 f(x) \, dx$.

**10.** The Midpoint rule for approximating $\int_{-1}^1 f(x) \, dx$ gives the value 12, the Composite Midpoint rule with $n = 2$ gives 5, and Composite Simpson's rule gives 6. Use the fact that $f(-1) = f(1)$ and $f(-0.5) = f(0.5) - 1$ to determine $f(-1)$, $f(-0.5)$, $f(0)$, $f(0.5)$, and $f(1)$.

**11.** Determine the values of $n$ and $h$ required to approximate

$$\int_0^2 e^{2x} \sin 3x \, dx$$

to within $10^{-4}$. Use

**a.** Composite Trapezoidal rule.

**b.** Composite Simpson's rule.

**c.** Composite Midpoint rule.

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**12.** Repeat Exercise 11 for the integral $\int_0^{\pi} x^2 \cos x \, dx$.

**13.** Determine the values of $n$ and $h$ required to approximate

$$\int_0^2 \frac{1}{x+4} \, dx$$

to within $10^{-5}$ and compute the approximation. Use

**a.** Composite Trapezoidal rule.

**b.** Composite Simpson's rule.

**c.** Composite Midpoint rule.

**14.** Repeat Exercise 13 for the integral $\int_1^2 x \ln x \, dx$.

**15.** Let $f$ be defined by

$$f(x) = \begin{cases} x^3 + 1, & 0 \le x \le 0.1, \\ 1.001 + 0.03(x-0.1) + 0.3(x-0.1)^2 + 2(x-0.1)^3, & 0.1 \le x \le 0.2, \\ 1.009 + 0.15(x-0.2) + 0.9(x-0.2)^2 + 2(x-0.2)^3, & 0.2 \le x \le 0.3. \end{cases}$$

**a.** Investigate the continuity of the derivatives of $f$.

**b.** Use the Composite Trapezoidal rule with $n = 6$ to approximate $\int_0^{0.3} f(x) \, dx$, and estimate the error using the error bound.

**c.** Use the Composite Simpson's rule with $n = 6$ to approximate $\int_0^{0.3} f(x) \, dx$. Are the results more accurate than in part (b)?

**16.** Show that the error $E(f)$ for Composite Simpson's rule can be approximated by

$$-\frac{h^4}{180}[f'''(b) - f'''(a)].$$

[*Hint:* $\sum_{j=1}^{n/2} f^{(4)}(\xi_j)(2h)$ is a Riemann Sum for $\int_a^b f^{(4)}(x) \, dx$.]

**17.** **a.** Derive an estimate for $E(f)$ in the Composite Trapezoidal rule using the method in Exercise 16.

**b.** Repeat part (a) for the Composite Midpoint rule.

**18.** Use the error estimates of Exercises 16 and 17 to estimate the errors in Exercise 12.

**19.** Use the error estimates of Exercises 16 and 17 to estimate the errors in Exercise 14.

**20.** In multivariable calculus and in statistics courses it is shown that

$$\int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} e^{-(1/2)(x/\sigma)^2} \, dx = 1,$$

for any positive $\sigma$. The function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(1/2)(x/\sigma)^2}$$

is the *normal density function* with *mean* $\mu = 0$ and *standard deviation* $\sigma$. The probability that a randomly chosen value described by this distribution lies in $[a, b]$ is given by $\int_a^b f(x) \, dx$. Approximate to within $10^{-5}$ the probability that a randomly chosen value described by this distribution will lie in

**a.** $[-\sigma, \sigma]$ **b.** $[-2\sigma, 2\sigma]$ **c.** $[-3\sigma, 3\sigma]$

**21.** Determine to within $10^{-6}$ the length of the graph of the ellipse with equation $4x^2 + 9y^2 = 36$.

**22.** A car laps a race track in 84 seconds. The speed of the car at each 6-second interval is determined by using a radar gun and is given from the beginning of the lap, in feet/second, by the entries in the following table.

| Time | 0 | 6 | 12 | 18 | 24 | 30 | 36 | 42 | 48 | 54 | 60 | 66 | 72 | 78 | 84 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Speed | 124 | 134 | 148 | 156 | 147 | 133 | 121 | 109 | 99 | 85 | 78 | 89 | 104 | 116 | 123 |

How long is the track?

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**23.** A particle of mass $m$ moving through a fluid is subjected to a viscous resistance $R$, which is a function of the velocity $v$. The relationship between the resistance $R$, velocity $v$, and time $t$ is given by the equation

$$t = \int_{v(t_0)}^{v(t)} \frac{m}{R(u)}\, du.$$

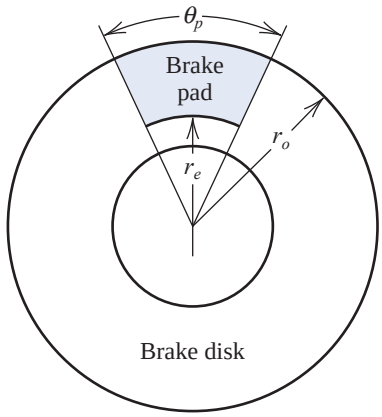
Suppose that $R(v) = -v\sqrt{v}$ for a particular fluid, where $R$ is in newtons and $v$ is in meters/second. If $m = 10$ kg and $v(0) = 10$ m/s, approximate the time required for the particle to slow to $v = 5$ m/s.

**24.** To simulate the thermal characteristics of disk brakes (see the following figure), D. A. Secrist and R. W. Hornbeck [SH] needed to approximate numerically the "area averaged lining temperature," $T$, of the brake pad from the equation

$$T = \frac{\displaystyle\int_{r_e}^{r_0} T(r) r\theta_p\, dr}{\displaystyle\int_{r_e}^{r_0} r\theta_p\, dr},$$

where $r_e$ represents the radius at which the pad-disk contact begins, $r_0$ represents the outside radius of the pad-disk contact, $\theta_p$ represents the angle subtended by the sector brake pads, and $T(r)$ is the temperature at each point of the pad, obtained numerically from analyzing the heat equation (see Section 12.2). Suppose $r_e = 0.308$ ft, $r_0 = 0.478$ ft, $\theta_p = 0.7051$ radians, and the temperatures given in the following table have been calculated at the various points on the disk. Approximate $T$.

| $r$ (ft) | $T(r)$ (°F) | $r$ (ft) | $T(r)$ (°F) | $r$ (ft) | $T(r)$ (°F) |
|---|---|---|---|---|---|
| 0.308 | 640 | 0.376 | 1034 | 0.444 | 1204 |
| 0.325 | 794 | 0.393 | 1064 | 0.461 | 1222 |
| 0.342 | 885 | 0.410 | 1114 | 0.478 | 1239 |
| 0.359 | 943 | 0.427 | 1152 | | |




**25.** Find an approximation to within $10^{-4}$ of the value of the integral considered in the application opening this chapter:

$$\int_0^{48} \sqrt{1 + (\cos x)^2}\, dx.$$

**26.** The equation

$$\int_0^x \frac{1}{\sqrt{2\pi}} e^{-t^2/2}\, dt = 0.45$$

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can be solved for $x$ by using Newton's method with

$$f(x) = \int_0^x \frac{1}{\sqrt{2\pi}} e^{-t^2/2}\, dt - 0.45$$

and

$$f'(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$

To evaluate $f$ at the approximation $p_k$, we need a quadrature formula to approximate

$$\int_0^{p_k} \frac{1}{\sqrt{2\pi}} e^{-t^2/2}\, dt.$$

**a.** Find a solution to $f(x) = 0$ accurate to within $10^{-5}$ using Newton's method with $p_0 = 0.5$ and the Composite Simpson's rule.

**b.** Repeat (a) using the Composite Trapezoidal rule in place of the Composite Simpson's rule.

## 4.5 Romberg Integration

In this section we will illustrate how Richardson extrapolation applied to results from the Composite Trapezoidal rule can be used to obtain high accuracy approximations with little computational cost.

In Section 4.4 we found that the Composite Trapezoidal rule has a truncation error of order $O(h^2)$. Specifically, we showed that for $h = (b-a)/n$ and $x_j = a + jh$ we have

$$\int_a^b f(x)\, dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{(b-a)f''(\mu)}{12}h^2.$$

for some number $\mu$ in $(a, b)$.

By an alternative method it can be shown (see [RR], pp. 136–140), that if $f \in C^\infty[a, b]$, the Composite Trapezoidal rule can also be written with an error term in the form

$$\int_a^b f(x)\, dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] + K_1h^2 + K_2h^4 + K_3h^6 + \cdots, \quad (4.33)$$

where each $K_i$ is a constant that depends only on $f^{(2i-1)}(a)$ and $f^{(2i-1)}(b)$.

Recall from Section 4.2 that Richardson extrapolation can be performed on any approximation procedure whose truncation error is of the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m}),$$

for a collection of constants $K_j$ and when $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$. In that section we gave demonstrations to illustrate how effective this techniques is when the approximation procedure has a truncation error with only even powers of $h$, that is, when the truncation error has the form.

$$\sum_{j=1}^{m-1} K_j h^{2j} + O(h^{2m}).$$

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Werner Romberg (1909–2003) devised this procedure for improving the accuracy of the Trapezoidal rule by eliminating the successive terms in the asymptotic expansion in 1955.

Because the Composite Trapezoidal rule has this form, it is an obvious candidate for extrapolation. This results in a technique known as **Romberg integration**.

To approximate the integral $\int_a^b f(x)\,dx$ we use the results of the Composite Trapezoidal rule with $n = 1, 2, 4, 8, 16, \ldots$, and denote the resulting approximations, respectively, by $R_{1,1}, R_{2,1}, R_{3,1}$, etc. We then apply extrapolation in the manner given in Section 4.2, that is, we obtain $O(h^4)$ approximations $R_{2,2}, R_{3,2}, R_{4,2}$, etc., by

$$R_{k,2} = R_{k,1} + \frac{1}{3}(R_{k,1} - R_{k-1,1}), \quad \text{for } k = 2, 3, \ldots$$

Then $O(h^6)$ approximations $R_{3,3}, R_{4,3}, R_{5,3}$, etc., by

$$R_{k,3} = R_{k,2} + \frac{1}{15}(R_{k,2} - R_{k-1,2}), \quad \text{for } k = 3, 4, \ldots.$$

In general, after the appropriate $R_{k,j-1}$ approximations have been obtained, we determine the $O(h^{2j})$ approximations from

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1} - 1}(R_{k,j-1} - R_{k-1,j-1}), \quad \text{for } k = j, j+1, \ldots$$

**Example 1** Use the Composite Trapezoidal rule to find approximations to $\int_0^{\pi} \sin x\,dx$ with $n = 1$, 2, 4, 8, and 16. Then perform Romberg extrapolation on the results.

The Composite Trapezoidal rule for the various values of $n$ gives the following approximations to the true value 2.

$$R_{1,1} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0;$$

$$R_{2,1} = \frac{\pi}{4}\left[\sin 0 + 2\sin\frac{\pi}{2} + \sin \pi\right] = 1.57079633;$$

$$R_{3,1} = \frac{\pi}{8}\left[\sin 0 + 2\left(\sin\frac{\pi}{4} + \sin\frac{\pi}{2} + \sin\frac{3\pi}{4}\right) + \sin \pi\right] = 1.89611890;$$

$$R_{4,1} = \frac{\pi}{16}\left[\sin 0 + 2\left(\sin\frac{\pi}{8} + \sin\frac{\pi}{4} + \cdots + \sin\frac{3\pi}{4} + \sin\frac{7\pi}{8}\right) + \sin \pi\right] = 1.97423160;$$

$$R_{5,1} = \frac{\pi}{32}\left[\sin 0 + 2\left(\sin\frac{\pi}{16} + \sin\frac{\pi}{8} + \cdots + \sin\frac{7\pi}{8} + \sin\frac{15\pi}{16}\right) + \sin \pi\right] = 1.99357034.$$

The $O(h^4)$ approximations are

$$R_{2,2} = R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1}) = 2.09439511; \quad R_{3,2} = R_{3,1} + \frac{1}{3}(R_{3,1} - R_{2,1}) = 2.00455976;$$

$$R_{4,2} = R_{4,1} + \frac{1}{3}(R_{4,1} - R_{3,1}) = 2.00026917; \quad R_{5,2} = R_{5,1} + \frac{1}{3}(R_{5,1} - R_{4,1}) = 2.00001659;$$

The $O(h^6)$ approximations are

$$R_{3,3} = R_{3,2} + \frac{1}{15}(R_{3,2} - R_{2,2}) = 1.99857073; \quad R_{4,3} = R_{4,2} + \frac{1}{15}(R_{4,2} - R_{3,2}) = 1.99998313;$$

$$R_{5,3} = R_{5,2} + \frac{1}{15}(R_{5,2} - R_{4,2}) = 1.99999975.$$

The two $O(h^8)$ approximations are

$$R_{4,4} = R_{4,3} + \frac{1}{63}(R_{4,3} - R_{3,3}) = 2.00000555; \quad R_{5,4} = R_{5,3} + \frac{1}{63}(R_{5,3} - R_{4,3}) = 2.00000001,$$

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and the final $O(h^{10})$ approximation is

$$R_{5,5} = R_{5,4} + \frac{1}{255}(R_{5,4} - R_{4,4}) = 1.99999999.$$

These results are shown in Table 4.9. ■

**Table 4.9**

| | | | | |
|---|---|---|---|---|
| 0 | | | | |
| 1.57079633 | 2.09439511 | | | |
| 1.89611890 | 2.00455976 | 1.99857073 | | |
| 1.97423160 | 2.00026917 | 1.99998313 | 2.00000555 | |
| 1.99357034 | 2.00001659 | 1.99999975 | 2.00000001 | 1.99999999 |

Notice that when generating the approximations for the Composite Trapezoidal rule approximations in Example 1, each consecutive approximation included all the functions evaluations from the previous approximation. That is, $R_{1,1}$ used evaluations at 0 and $\pi$, $R_{2,1}$ used these evaluations and added an evaluation at the intermediate point $\pi/2$. Then $R_{3,1}$ used the evaluations of $R_{2,1}$ and added two additional intermediate ones at $\pi/4$ and $3\pi/4$. This pattern continues with $R_{4,1}$ using the same evaluations as $R_{3,1}$ but adding evaluations at the 4 intermediate points $\pi/8$, $3\pi/8$, $5\pi/8$, and $7\pi/8$, and so on.

This evaluation procedure for Composite Trapezoidal rule approximations holds for an integral on any interval $[a, b]$. In general, the Composite Trapezoidal rule denoted $R_{k+1,1}$ uses the same evaluations as $R_{k,1}$ but adds evaluations at the $2^{k-2}$ intermediate points. Efficient calculation of these approximations can therefore be done in a recursive manner.

To obtain the Composite Trapezoidal rule approximations for $\int_a^b f(x)\,dx$, let $h_k = (b-a)/m_k = (b-a)/2^{k-1}$. Then

$$R_{1,1} = \frac{h_1}{2}[f(a) + f(b)] = \frac{(b-a)}{2}[f(a) + f(b)];$$

and

$$R_{2,1} = \frac{h_2}{2}[f(a) + f(b) + 2f(a + h_2)].$$

By reexpressing this result for $R_{2,1}$ we can incorporate the previously determined approximation $R_{1,1}$

$$R_{2,1} = \frac{(b-a)}{4}\left[f(a) + f(b) + 2f\left(a + \frac{(b-a)}{2}\right)\right] = \frac{1}{2}[R_{1,1} + h_1 f(a + h_2)].$$

In a similar manner we can write

$$R_{3,1} = \frac{1}{2}\{R_{2,1} + h_2[f(a + h_3) + f(a + 3h_3)]\};$$

and, in general (see Figure 4.10 on page 216), we have

$$R_{k,1} = \frac{1}{2}\left[R_{k-1,1} + h_{k-1}\sum_{i=1}^{2^{k-2}} f\,(a + (2i-1)h_k)\right], \tag{4.34}$$

for each $k = 2, 3, \ldots, n$. (See Exercises 14 and 15.)

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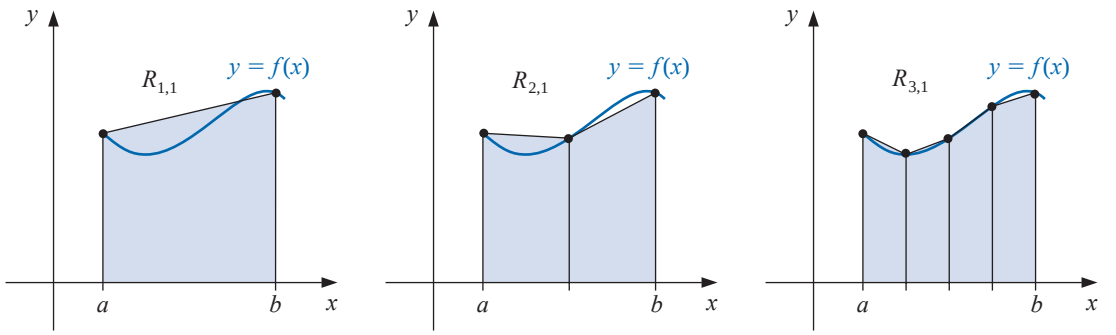
**Figure 4.10**




Extrapolation then is used to produce $O(h_k^{2j})$ approximations by

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1} - 1}(R_{k,j-1} - R_{k-1,j-1}), \quad \text{for } k = j, j+1, \ldots$$

as shown in Table 4.10.

**Table 4.10**

| $k$ | $O(h_k^2)$ | $O(h_k^4)$ | $O(h_k^6)$ | $O(h_k^8)$ | | $O(h_k^{2n})$ |
|---|---|---|---|---|---|---|
| 1 | $R_{1,1}$ | | | | | |
| 2 | $R_{2,1}$ | $R_{2,2}$ | | | | |
| 3 | $R_{3,1}$ | $R_{3,2}$ | $R_{3,3}$ | | | |
| 4 | $R_{4,1}$ | $R_{4,2}$ | $R_{4,3}$ | $R_{4,4}$ | | |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ | |
| $n$ | $R_{n,1}$ | $R_{n,2}$ | $R_{n,3}$ | $R_{n,4}$ | $\cdots$ | $R_{n,n}$ |

The effective method to construct the Romberg table makes use of the highest order of approximation at each step. That is, it calculates the entries row by row, in the order $R_{1,1}$, $R_{2,1}$, $R_{2,2}$, $R_{3,1}$, $R_{3,2}$, $R_{3,3}$, etc. This also permits an entire new row in the table to be calculated by doing only one additional application of the Composite Trapezoidal rule. It then uses a simple averaging on the previously calculated values to obtain the remaining entries in the row. Remember

- Calculate the Romberg table one complete row at a time.

**Example 2** Add an additional extrapolation row to Table 4.10 to approximate $\int_0^{\pi} \sin x \, dx$.

***Solution*** To obtain the additional row we need the trapezoidal approximation

$$R_{6,1} = \frac{1}{2}\left[R_{5,1} + \frac{\pi}{16}\sum_{k=1}^{2^4} \sin\frac{(2k-1)\pi}{32}\right] = 1.99839336.$$

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The values in Table 4.10 give

$$R_{6,2} = R_{6,1} + \frac{1}{3}(R_{6,1} - R_{5,1}) = 1.99839336 + \frac{1}{3}(1.99839336 - 1.99357035)$$
$$= 2.00000103;$$
$$R_{6,3} = R_{6,2} + \frac{1}{15}(R_{6,2} - R_{5,2}) = 2.00000103 + \frac{1}{15}(2.00000103 - 2.00001659)$$
$$= 2.00000000;$$
$$R_{6,4} = R_{6,3} + \frac{1}{63}(R_{6,3} - R_{5,3}) = 2.00000000;$$
$$R_{6,5} = R_{6,4} + \frac{1}{255}(R_{6,4} - R_{5,4}) = 2.00000000;$$

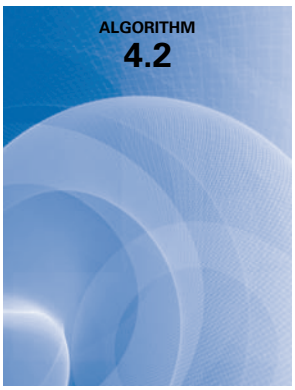
and $R_{6,6} = R_{6,5} + \frac{1}{1023}(R_{6,5} - R_{5,5}) = 2.00000000$. The new extrapolation table is shown in Table 4.11. ■

**Table 4.11**

| | | | | | |
|---|---|---|---|---|---|
| 0 | | | | | |
| 1.57079633 | 2.09439511 | | | | |
| 1.89611890 | 2.00455976 | 1.99857073 | | | |
| 1.97423160 | 2.00026917 | 1.99998313 | 2.00000555 | | |
| 1.99357034 | 2.00001659 | 1.99999975 | 2.00000001 | 1.99999999 | |
| 1.99839336 | 2.00000103 | 2.00000000 | 2.00000000 | 2.00000000 | 2.00000000 |

Notice that all the extrapolated values except for the first (in the first row of the second column) are more accurate than the best composite trapezoidal approximation (in the last row of the first column). Although there are 21 entries in Table 4.11, only the six in the left column require function evaluations since these are the only entries generated by the Composite Trapezoidal rule; the other entries are obtained by an averaging process. In fact, because of the recurrence relationship of the terms in the left column, the only function evaluations needed are those to compute the final Composite Trapezoidal rule approximation. In general, $R_{k,1}$ requires $1 + 2^{k-1}$ function evaluations, so in this case $1 + 2^5 = 33$ are needed.

Algorithm 4.2 uses the recursive procedure to find the initial Composite Trapezoidal Rule approximations and computes the results in the table row by row.




## Romberg

To approximate the integral $I = \int_a^b f(x)\,dx$, select an integer $n > 0$.

**INPUT** endpoints $a, b$; integer $n$.

**OUTPUT** an array $R$. (*Compute R by rows; only the last 2 rows are saved in storage.*)

***Step 1*** Set $h = b - a$;
$R_{1,1} = \frac{h}{2}(f(a) + f(b))$.

***Step 2*** OUTPUT $(R_{1,1})$.

***Step 3*** For $i = 2, \ldots, n$ do Steps 4–8.

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**Step 4** Set $R_{2,1} = \frac{1}{2}\left[R_{1,1} + h\sum_{k=1}^{2^{i-2}} f(a + (k - 0.5)h)\right]$.

(*Approximation from Trapezoidal method.*)

**Step 5** For $j = 2, \ldots, i$

set $R_{2,j} = R_{2,j-1} + \frac{R_{2,j-1} - R_{1,j-1}}{4^{j-1} - 1}$. (*Extrapolation.*)

**Step 6** OUTPUT ($R_{2,j}$ for $j = 1, 2, \ldots, i$).

**Step 7** Set $h = h/2$.

**Step 8** For $j = 1, 2, \ldots, i$ set $R_{1,j} = R_{2,j}$. (*Update row 1 of R.*)

**Step 9** STOP. ■

Algorithm 4.2 requires a preset integer $n$ to determine the number of rows to be generated. We could also set an error tolerance for the approximation and generate $n$, within some upper bound, until consecutive diagonal entries $R_{n-1,n-1}$ and $R_{n,n}$ agree to within the tolerance. To guard against the possibility that two consecutive row elements agree with each other but not with the value of the integral being approximated, it is common to generate approximations until not only $|R_{n-1,n-1} - R_{n,n}|$ is within the tolerance, but also $|R_{n-2,n-2} - R_{n-1,n-1}|$. Although not a universal safeguard, this will ensure that two differently generated sets of approximations agree within the specified tolerance before $R_{n,n}$, is accepted as sufficiently accurate.

Romberg integration can be performed with the *Quadrature* command in the *NumericalAnalysis* subpackage of Maple's *Student* package. For example, after loading the package and defining the function and interval, the command

$$Quadrature(f(x), x = a..b, method = romberg_6, output = information)$$

produces the values shown in Table 4.11 together with the information that 6 applications of the Trapezoidal rule were used and 33 function evaluations were required.

Romberg integration applied to a function $f$ on the interval $[a, b]$ relies on the assumption that the Composite Trapezoidal rule has an error term that can be expressed in the form of Eq. (4.33); that is, we must have $f \in C^{2k+2}[a, b]$ for the $k$th row to be generated. General-purpose algorithms using Romberg integration include a check at each stage to ensure that this assumption is fulfilled. These methods are known as *cautious Romberg algorithms* and are described in [Joh]. This reference also describes methods for using the Romberg technique as an adaptive procedure, similar to the adaptive Simpson's rule that will be discussed in Section 4.6.

The adjective *cautious* used in the description of a numerical method indicates that a check is incorporated to determine if the continuity hypotheses are likely to be true.

## EXERCISE SET 4.5

**1.** Use Romberg integration to compute $R_{3,3}$ for the following integrals.

**a.** $\int_1^{1.5} x^2 \ln x \, dx$

**b.** $\int_0^1 x^2 e^{-x} \, dx$

**c.** $\int_0^{0.35} \frac{2}{x^2 - 4} \, dx$

**d.** $\int_0^{\pi/4} x^2 \sin x \, dx$

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**e.** $\int_0^{\pi/4} e^{3x} \sin 2x \, dx$ **f.** $\int_1^{1.6} \frac{2x}{x^2 - 4} \, dx$

**g.** $\int_3^{3.5} \frac{x}{\sqrt{x^2 - 4}} \, dx$ **h.** $\int_0^{\pi/4} (\cos x)^2 \, dx$

**2.** Use Romberg integration to compute $R_{3,3}$ for the following integrals.

**a.** $\int_{-1}^{1} (\cos x)^2 \, dx$ **b.** $\int_{-0.75}^{0.75} x \ln(x + 1) \, dx$

**c.** $\int_1^4 \left((\sin x)^2 - 2x \sin x + 1\right) \, dx$ **d.** $\int_e^{2e} \frac{1}{x \ln x} \, dx$

**3.** Calculate $R_{4,4}$ for the integrals in Exercise 1.

**4.** Calculate $R_{4,4}$ for the integrals in Exercise 2.

**5.** Use Romberg integration to approximate the integrals in Exercise 1 to within $10^{-6}$. Compute the Romberg table until either $|R_{n-1,n-1} - R_{n,n}| < 10^{-6}$, or $n = 10$. Compare your results to the exact values of the integrals.

**6.** Use Romberg integration to approximate the integrals in Exercise 2 to within $10^{-6}$. Compute the Romberg table until either $|R_{n-1,n-1} - R_{n,n}| < 10^{-6}$, or $n = 10$. Compare your results to the exact values of the integrals.

**7.** Use the following data to approximate $\int_1^5 f(x) \, dx$ as accurately as possible.

| $x$ | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| $f(x)$ | 2.4142 | 2.6734 | 2.8974 | 3.0976 | 3.2804 |

**8.** Romberg integration is used to approximate

$$\int_0^1 \frac{x^2}{1 + x^3} \, dx.$$

If $R_{11} = 0.250$ and $R_{22} = 0.2315$, what is $R_{21}$?

**9.** Romberg integration is used to approximate

$$\int_2^3 f(x) \, dx.$$

If $f(2) = 0.51342$, $f(3) = 0.36788$, $R_{31} = 0.43687$, and $R_{33} = 0.43662$, find $f(2.5)$.

**10.** Romberg integration for approximating $\int_0^1 f(x) \, dx$ gives $R_{11} = 4$ and $R_{22} = 5$. Find $f(1/2)$.

**11.** Romberg integration for approximating $\int_a^b f(x) \, dx$ gives $R_{11} = 8$, $R_{22} = 16/3$, and $R_{33} = 208/45$. Find $R_{31}$.

**12.** Use Romberg integration to compute the following approximations to

$$\int_0^{48} \sqrt{1 + (\cos x)^2} \, dx.$$

[*Note:* The results in this exercise are most interesting if you are using a device with between seven- and nine-digit arithmetic.]

**a.** Determine $R_{1,1}$, $R_{2,1}$, $R_{3,1}$, $R_{4,1}$, and $R_{5,1}$, and use these approximations to predict the value of the integral.

**b.** Determine $R_{2,2}$, $R_{3,3}$, $R_{4,4}$, and $R_{5,5}$, and modify your prediction.

**c.** Determine $R_{6,1}$, $R_{6,2}$, $R_{6,3}$, $R_{6,4}$, $R_{6,5}$, and $R_{6,6}$, and modify your prediction.

**d.** Determine $R_{7,7}$, $R_{8,8}$, $R_{9,9}$, and $R_{10,10}$, and make a final prediction.

**e.** Explain why this integral causes difficulty with Romberg integration and how it can be reformulated to more easily determine an accurate approximation.

**13.** Show that the approximation obtained from $R_{k,2}$ is the same as that given by the Composite Simpson's rule described in Theorem 4.4 with $h = h_k$.

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**14.** Show that, for any $k$,

$$\sum_{i=1}^{2^{k-1}-1} f\left(a+\frac{i}{2}h_{k-1}\right) = \sum_{i=1}^{2^{k-2}} f\left(a+\left(i-\frac{1}{2}\right)h_{k-1}\right) + \sum_{i=1}^{2^{k-2}-1} f(a+ih_{k-1}).$$

**15.** Use the result of Exercise 14 to verify Eq. (4.34); that is, show that for all $k$,

$$R_{k,1} = \frac{1}{2}\left[R_{k-1,1} + h_{k-1}\sum_{i=1}^{2^{k-2}} f\left(a+\left(i-\frac{1}{2}\right)h_{k-1}\right)\right].$$

**16.** In Exercise 26 of Section 1.1, a Maclaurin series was integrated to approximate erf(1), where erf($x$) is the normal distribution error function defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt.$$

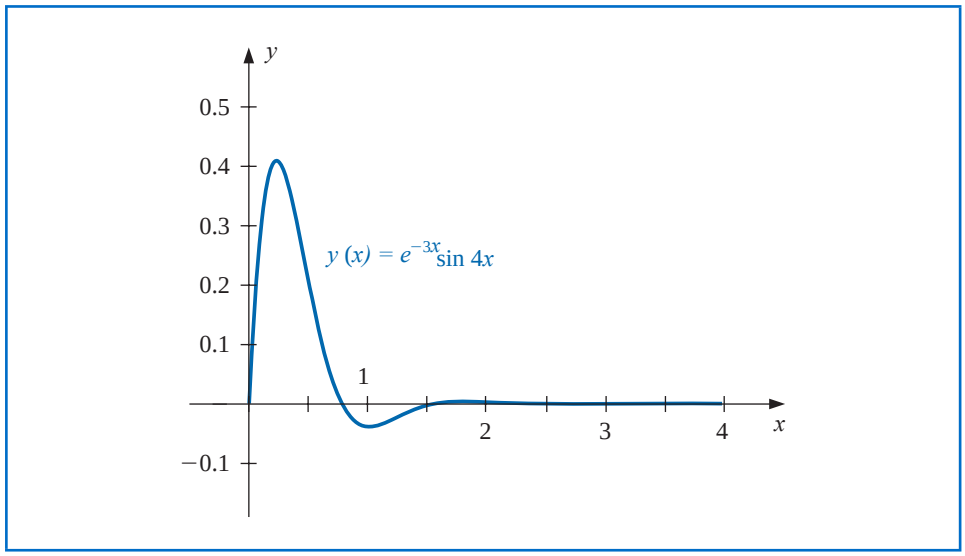
Approximate erf(1) to within $10^{-7}$.

## 4.6 Adaptive Quadrature Methods

The composite formulas are very effective in most situations, but they suffer occasionally because they require the use of equally-spaced nodes. This is inappropriate when integrating a function on an interval that contains both regions with large functional variation and regions with small functional variation.

**Illustration** The unique solution to the differential equation $y'' + 6y' + 25 = 0$ that additionally satisfies $y(0) = 0$ and $y'(0) = 4$ is $y(x) = e^{-3x}\sin 4x$. Functions of this type are common in mechanical engineering because they describe certain features of spring and shock absorber systems, and in electrical engineering because they are common solutions to elementary circuit problems. The graph of $y(x)$ for $x$ in the interval $[0, 4]$ is shown in Figure 4.11.

**Figure 4.11**

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Suppose that we need the integral of $y(x)$ on $[0, 4]$. The graph indicates that the integral on $[3, 4]$ must be very close to 0, and on $[2, 3]$ would also not be expected to be large. However, on $[0, 2]$ there is significant variation of the function and it is not at all clear what the integral is on this interval. This is an example of a situation where composite integration would be inappropriate. A very low order method could be used on $[2, 4]$, but a higher-order method would be necessary on $[0, 2]$. □

The question we will consider in this section is:

- How can we determine what technique should be applied on various portions of the interval of integration, and how accurate can we expect the final approximation to be?

We will see that under quite reasonable conditions we can answer this question and also determine approximations that satisfy given accuracy requirements.

If the approximation error for an integral on a given interval is to be evenly distributed, a smaller step size is needed for the large-variation regions than for those with less variation. An efficient technique for this type of problem should predict the amount of functional variation and adapt the step size as necessary. These methods are called **Adaptive quadrature methods**. Adaptive methods are particularly popular for inclusion in professional software packages because, in addition to being efficient, they generally provide approximations that are within a given specified tolerance.

In this section we consider an Adaptive quadrature method and see how it can be used to reduce approximation error and also to predict an error estimate for the approximation that does not rely on knowledge of higher derivatives of the function. The method we discuss is based on the Composite Simpson's rule, but the technique is easily modified to use other composite procedures.

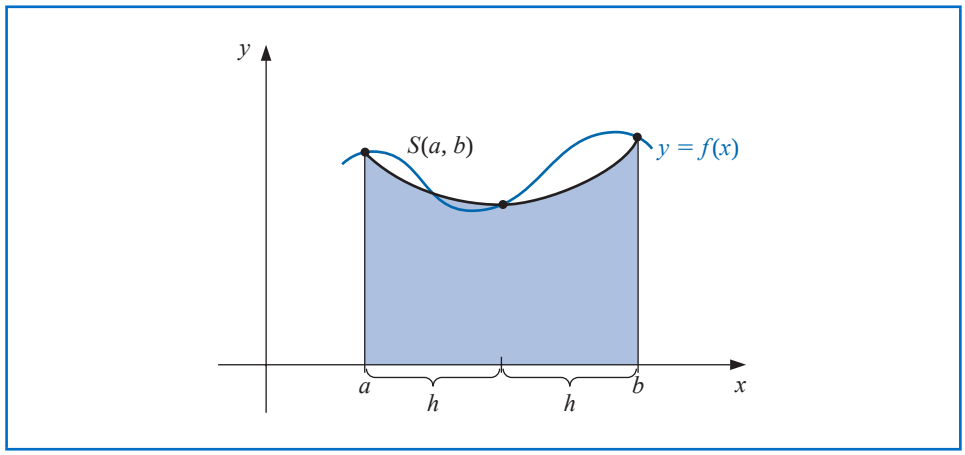
Suppose that we want to approximate $\int_a^b f(x)\,dx$ to within a specified tolerance $\varepsilon > 0$. The first step is to apply Simpson's rule with step size $h = (b - a)/2$. This produces (see Figure 4.12)

$$\int_a^b f(x)\,dx = S(a, b) - \frac{h^5}{90} f^{(4)}(\xi), \quad \text{for some } \xi \text{ in } (a, b), \tag{4.35}$$

where we denote the Simpson's rule approximation on $[a, b]$ by

$$S(a, b) = \frac{h}{3}[f(a) + 4f(a + h) + f(b)].$$

**Figure 4.12**

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The next step is to determine an accuracy approximation that does not require $f^{(4)}(\xi)$. To do this, we apply the Composite Simpson's rule with $n = 4$ and step size $(b-a)/4 = h/2$, giving

$$\int_a^b f(x)\,dx = \frac{h}{6}\left[f(a) + 4f\left(a + \frac{h}{2}\right) + 2f(a+h) + 4f\left(a + \frac{3h}{2}\right) + f(b)\right] - \left(\frac{h}{2}\right)^4 \frac{(b-a)}{180} f^{(4)}(\tilde{\xi}), \tag{4.36}$$

for some $\tilde{\xi}$ in $(a, b)$. To simplify notation, let

$$S\left(a, \frac{a+b}{2}\right) = \frac{h}{6}\left[f(a) + 4f\left(a + \frac{h}{2}\right) + f(a+h)\right]$$

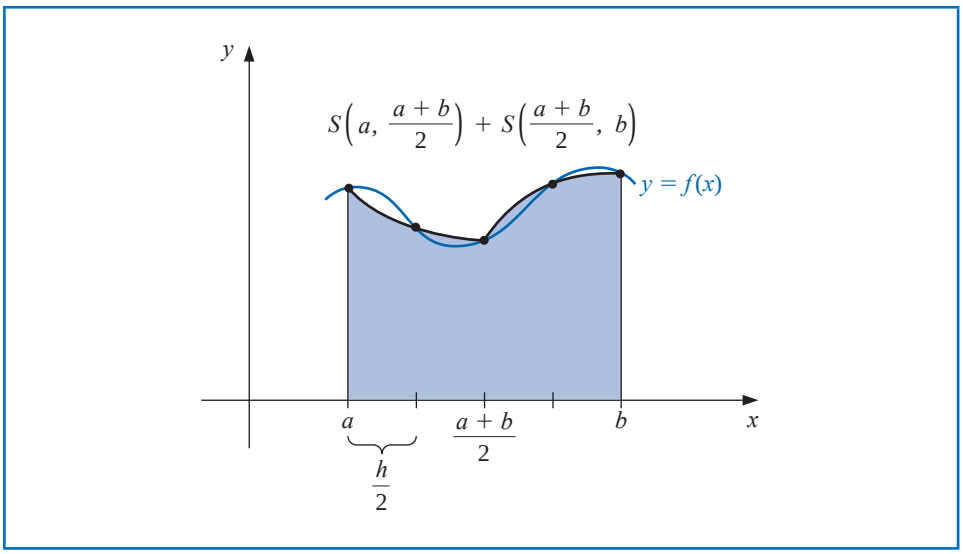
and

$$S\left(\frac{a+b}{2}, b\right) = \frac{h}{6}\left[f(a+h) + 4f\left(a + \frac{3h}{2}\right) + f(b)\right].$$

Then Eq. (4.36) can be rewritten (see Figure 4.13) as

$$\int_a^b f(x)\,dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\xi}). \tag{4.37}$$

**Figure 4.13**




The error estimation is derived by assuming that $\xi \approx \tilde{\xi}$ or, more precisely, that $f^{(4)}(\xi) \approx f^{(4)}(\tilde{\xi})$, and the success of the technique depends on the accuracy of this assumption. If it is accurate, then equating the integrals in Eqs. (4.35) and (4.37) gives

$$S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\xi),$$

so

$$\frac{h^5}{90} f^{(4)}(\xi) \approx \frac{16}{15}\left[S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right].$$

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Using this estimate in Eq. (4.37) produces the error estimation

$$\left|\int_a^b f(x)\,dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \approx \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi)$$
$$\approx \frac{1}{15}\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right|.$$

This implies that $S(a,(a+b)/2)+S((a+b)/2,b)$ approximates $\int_a^b f(x)\,dx$ about 15 times better than it agrees with the computed value $S(a,b)$. Thus, if

$$\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < 15\varepsilon, \tag{4.38}$$

we expect to have

$$\left|\int_a^b f(x)\,dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < \varepsilon, \tag{4.39}$$

and

$$S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$$

is assumed to be a sufficiently accurate approximation to $\int_a^b f(x)\,dx$.

**Example 1** Check the accuracy of the error estimate given in (4.38) and (4.39) when applied to the integral

$$\int_0^{\pi/2} \sin x\,dx = 1.$$

by comparing

$$\frac{1}{15}\left|S\left(0, \frac{\pi}{2}\right) - S\left(0, \frac{\pi}{4}\right) - S\left(\frac{\pi}{4}, \frac{\pi}{2}\right)\right| \quad \text{to} \quad \left|\int_0^{\pi/2} \sin x\,dx - S\left(0, \frac{\pi}{4}\right) - S\left(\frac{\pi}{4}, \frac{\pi}{2}\right)\right|.$$

***Solution*** We have

$$S\left(0, \frac{\pi}{2}\right) = \frac{\pi/4}{3}\left[\sin 0 + 4\sin\frac{\pi}{4} + \sin\frac{\pi}{2}\right] = \frac{\pi}{12}(2\sqrt{2}+1) = 1.002279878$$

and

$$S\left(0, \frac{\pi}{4}\right) + S\left(\frac{\pi}{4}, \frac{\pi}{2}\right) = \frac{\pi/8}{3}\left[\sin 0 + 4\sin\frac{\pi}{8} + 2\sin\frac{\pi}{4} + 4\sin\frac{3\pi}{8} + \sin\frac{\pi}{2}\right]$$
$$= 1.000134585.$$

So

$$\left|S\left(0, \frac{\pi}{2}\right) - S\left(0, \frac{\pi}{4}\right) - S\left(\frac{\pi}{4}, \frac{\pi}{2}\right)\right| = |1.002279878 - 1.000134585| = 0.002145293.$$

The estimate for the error obtained when using $S(a,(a+b))+S((a+b),b)$ to approximate $\int_a^b f(x)\,dx$ is consequently

$$\frac{1}{15}\left|S\left(0, \frac{\pi}{2}\right) - S\left(0, \frac{\pi}{4}\right) - S\left(\frac{\pi}{4}, \frac{\pi}{2}\right)\right| = 0.000143020,$$

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which closely approximates the actual error

$$\left| \int_0^{\pi/2} \sin x \, dx - 1.000134585 \right| = 0.000134585,$$

even though $D_x^4 \sin x = \sin x$ varies significantly in the interval $(0, \pi/2)$. ■

When the approximations in (4.38) differ by more than $15\varepsilon$, we can apply the Simpson's rule technique individually to the subintervals $[a, (a+b)/2]$ and $[(a+b)/2, b]$. Then we use the error estimation procedure to determine if the approximation to the integral on each subinterval is within a tolerance of $\varepsilon/2$. If so, we sum the approximations to produce an approximation to $\int_a^b f(x)\,dx$ within the tolerance $\varepsilon$.

If the approximation on one of the subintervals fails to be within the tolerance $\varepsilon/2$, then that subinterval is itself subdivided, and the procedure is reapplied to the two subintervals to determine if the approximation on each subinterval is accurate to within $\varepsilon/4$. This halving procedure is continued until each portion is within the required tolerance.

Problems can be constructed for which this tolerance will never be met, but the technique is usually successful, because each subdivision typically increases the accuracy of the approximation by a factor of 16 while requiring an increased accuracy factor of only 2.

Algorithm 4.3 details this Adaptive quadrature procedure for Simpson's rule, although some technical difficulties arise that require the implementation to differ slightly from the preceding discussion. For example, in Step 1 the tolerance has been set at $10\varepsilon$ rather than the $15\varepsilon$ figure in Inequality (4.38). This bound is chosen conservatively to compensate for error in the assumption $f^{(4)}(\xi) \approx f^{(4)}(\tilde{\xi})$. In problems where $f^{(4)}$ is known to be widely varying, this bound should be decreased even further.

It is a good idea to include a margin of safety when it is impossible to verify accuracy assumptions.

The procedure listed in the algorithm first approximates the integral on the leftmost subinterval in a subdivision. This requires the efficient storing and recalling of previously computed functional evaluations for the nodes in the right half subintervals. Steps 3, 4, and 5 contain a stacking procedure with an indicator to keep track of the data that will be required for calculating the approximation on the subinterval immediately adjacent and to the right of the subinterval on which the approximation is being generated. The method is easier to implement using a recursive programming language.

## Adaptive Quadrature

To approximate the integral $I = \int_a^b f(x)\,dx$ to within a given tolerance:

INPUT endpoints $a, b$; tolerance $TOL$; limit $N$ to number of levels.

OUTPUT approximation $APP$ or message that $N$ is exceeded.

*Step 1* Set $APP = 0$;
$i = 1$;
$TOL_i = 10\,TOL$;
$a_i = a$;
$h_i = (b-a)/2$;
$FA_i = f(a)$;
$FC_i = f(a + h_i)$;
$FB_i = f(b)$;
$S_i = h_i(FA_i + 4FC_i + FB_i)/3$; (*Approximation from Simpson's method for entire interval.*)
$L_i = 1$.

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*Step 2* While $i > 0$ do Steps 3–5.

*Step 3* Set $FD = f(a_i + h_i/2)$;
$FE = f(a_i + 3h_i/2)$;
$S1 = h_i(FA_i + 4FD + FC_i)/6$; (*Approximations from Simpson's method for halves of subintervals.*)
$S2 = h_i(FC_i + 4FE + FB_i)/6$;
$v_1 = a_i$; (*Save data at this level.*)
$v_2 = FA_i$;
$v_3 = FC_i$;
$v_4 = FB_i$;
$v_5 = h_i$;
$v_6 = TOL_i$;
$v_7 = S_i$;
$v_8 = L_i$.

*Step 4* Set $i = i - 1$. (*Delete the level.*)

*Step 5* If $|S1 + S2 - v_7| < v_6$
then set $APP = APP + (S1 + S2)$
else
if $(v_8 \geq N)$
then
OUTPUT ('LEVEL EXCEEDED'); (*Procedure fails.*)
STOP.
else (*Add one level.*)
set $i = i + 1$; (*Data for right half subinterval.*)
$a_i = v_1 + v_5$;
$FA_i = v_3$;
$FC_i = FE$;
$FB_i = v_4$;
$h_i = v_5/2$;
$TOL_i = v_6/2$;
$S_i = S2$;
$L_i = v_8 + 1$;
set $i = i + 1$; (*Data for left half subinterval.*)
$a_i = v_1$;
$FA_i = v_2$;
$FC_i = FD$;
$FB_i = v_3$;
$h_i = h_{i-1}$;
$TOL_i = TOL_{i-1}$;
$S_i = S1$;
$L_i = L_{i-1}$.

*Step 6* OUTPUT ($APP$); (*$APP$ approximates $I$ to within $TOL$.*)
STOP. ■

**Illustration** The graph of the function $f(x) = (100/x^2)\sin(10/x)$ for $x$ in $[1, 3]$ is shown in Figure 4.14. Using the Adaptive Quadrature Algorithm 4.3 with tolerance $10^{-4}$ to approximate $\int_1^3 f(x)\,dx$ produces $-1.426014$, a result that is accurate to within $1.1 \times 10^{-5}$. The approximation required that Simpson's rule with $n = 4$ be performed on the 23 subintervals whose

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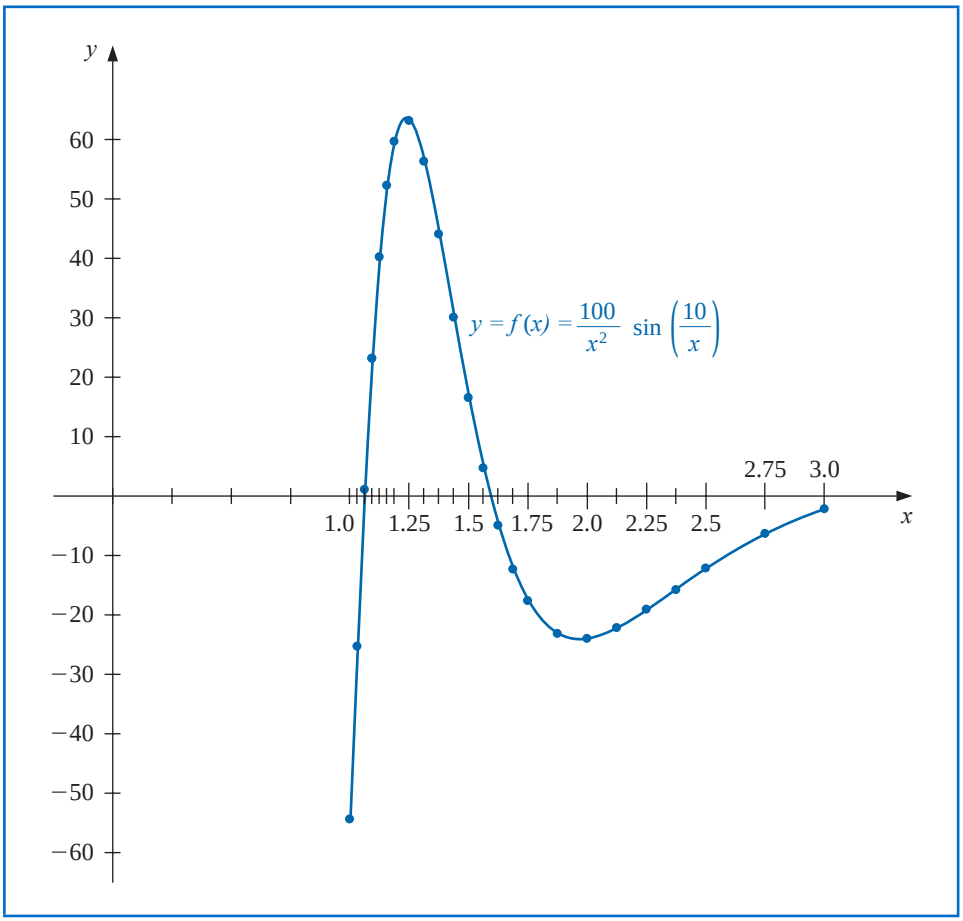
endpoints are shown on the horizontal axis in Figure 4.14. The total number of functional evaluations required for this approximation is 93.

**Figure 4.14**




The largest value of $h$ for which the standard Composite Simpson's rule gives $10^{-4}$ accuracy is $h = 1/88$. This application requires 177 function evaluations, nearly twice as many as Adaptive quadrature. □

Adaptive quadrature can be performed with the *Quadrature* command in the *NumericalAnalysis* subpackage of Maple's *Student* package. In this situation the option *adaptive* = *true* is used. For example, to produce the values in the Illustration we first load the package and define the function and interval with

$$f := x \to \frac{100}{x^2} \cdot \sin\left(\frac{10}{x}\right);\ a := 1.0;\ b := 3.0$$

Then give the *NumericalAnalysis* command

$$Quadrature(f(x), x = a..b, adaptive = true, method = [simpson, 10^{-4}], output = information)$$

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This produces the approximation $-1.42601481$ and a table that lists all the intervals on which Simpson's rule was employed and whether the appropriate tolerance was satisfied (indicated by the word `PASS`) or was not satisfied (indicated by the word `fail`). It also gives what Maple thinks is the correct value of the integral to the decimal places listed, in this case $-1.42602476$. Then it gives the absolute and relative errors, $9.946 \times 10^{-6}$ and $6.975 \times 10^{-4}$, respectively, assuming that its correct value is accurate.

## EXERCISE SET 4.6

**1.** Compute the Simpson's rule approximations $S(a, b)$, $S(a, (a + b)/2)$, and $S((a + b)/2, b)$ for the following integrals, and verify the estimate given in the approximation formula.

**a.** $\displaystyle\int_1^{1.5} x^2 \ln x \, dx$

**b.** $\displaystyle\int_0^1 x^2 e^{-x} \, dx$

**c.** $\displaystyle\int_0^{0.35} \frac{2}{x^2 - 4} \, dx$

**d.** $\displaystyle\int_0^{\pi/4} x^2 \sin x \, dx$

**e.** $\displaystyle\int_0^{\pi/4} e^{3x} \sin 2x \, dx$

**f.** $\displaystyle\int_1^{1.6} \frac{2x}{x^2 - 4} \, dx$

**g.** $\displaystyle\int_3^{3.5} \frac{x}{\sqrt{x^2 - 4}} \, dx$

**h.** $\displaystyle\int_0^{\pi/4} (\cos x)^2 \, dx$

**2.** Use Adaptive quadrature to find approximations to within $10^{-3}$ for the integrals in Exercise 1. Do not use a computer program to generate these results.

**3.** Use Adaptive quadrature to approximate the following integrals to within $10^{-5}$.

**a.** $\displaystyle\int_1^3 e^{2x} \sin 3x \, dx$

**b.** $\displaystyle\int_1^3 e^{3x} \sin 2x \, dx$

**c.** $\displaystyle\int_0^5 \left(2x \cos(2x) - (x - 2)^2\right) \, dx$

**d.** $\displaystyle\int_0^5 \left(4x \cos(2x) - (x - 2)^2\right) \, dx$

**4.** Use Adaptive quadrature to approximate the following integrals to within $10^{-5}$.

**a.** $\displaystyle\int_0^{\pi} (\sin x + \cos x) \, dx$

**b.** $\displaystyle\int_1^2 (x + \sin 4x) \, dx$

**c.** $\displaystyle\int_{-1}^1 x \sin 4x \, dx$

**d.** $\displaystyle\int_0^{\pi/2} (6 \cos 4x + 4 \sin 6x) e^x \, dx$

**5.** Use Simpson's Composite rule with $n = 4, 6, 8, \ldots$, until successive approximations to the following integrals agree to within $10^{-6}$. Determine the number of nodes required. Use the Adaptive Quadrature Algorithm to approximate the integral to within $10^{-6}$, and count the number of nodes. Did Adaptive quadrature produce any improvement?

**a.** $\displaystyle\int_0^{\pi} x \cos x^2 \, dx$

**b.** $\displaystyle\int_0^{\pi} x \sin x^2 \, dx$

**c.** $\displaystyle\int_0^{\pi} x^2 \cos x \, dx$

**d.** $\displaystyle\int_0^{\pi} x^2 \sin x \, dx$

**6.** Sketch the graphs of $\sin(1/x)$ and $\cos(1/x)$ on $[0.1, 2]$. Use Adaptive quadrature to approximate the following integrals to within $10^{-3}$.

**a.** $\displaystyle\int_{0.1}^2 \sin \frac{1}{x} \, dx$

**b.** $\displaystyle\int_{0.1}^2 \cos \frac{1}{x} \, dx$

**7.** The differential equation

$$mu''(t) + ku(t) = F_0 \cos \omega t$$

describes a spring-mass system with mass $m$, spring constant $k$, and no applied damping. The term $F_0 \cos \omega t$ describes a periodic external force applied to the system. The solution to the equation when the system is initially at rest ($u'(0) = u(0) = 0$) is

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$$u(t) = \frac{F_0}{m(\omega_0^2 - \omega^2)}(\cos \omega t - \cos \omega_0 t), \quad \text{where} \quad \omega_0 = \sqrt{\frac{k}{m}} \neq \omega.$$

Sketch the graph of $u$ when $m = 1$, $k = 9$, $F_0 = 1$, $\omega = 2$, and $t \in [0, 2\pi]$. Approximate $\int_0^{2\pi} u(t)\,dt$ to within $10^{-4}$.

**8.** If the term $cu'(t)$ is added to the left side of the motion equation in Exercise 7, the resulting differential equation describes a spring-mass system that is damped with damping constant $c \neq 0$. The solution to this equation when the system is initially at rest is

$$u(t) = c_1 e^{r_1 t} + c_2 e^{r_2 t} + \frac{F_0}{c^2\omega^2 + m^2(\omega_0^2 - \omega^2)^2}\left(c\omega \sin \omega t + m\left(\omega_0^2 - \omega^2\right)\cos \omega t\right),$$

where

$$r_1 = \frac{-c + \sqrt{c^2 - 4\omega_0^2 m^2}}{2m} \quad \text{and} \quad r_2 = \frac{-c - \sqrt{c^2 - 4\omega_0^2 m^2}}{2m}.$$

**a.** Let $m = 1$, $k = 9$, $F_0 = 1$, $c = 10$, and $\omega = 2$. Find the values of $c_1$ and $c_2$ so that $u(0) = u'(0) = 0$.

**b.** Sketch the graph of $u(t)$ for $t \in [0, 2\pi]$ and approximate $\int_0^{2\pi} u(t)\,dt$ to within $10^{-4}$.

**9.** Let $T(a, b)$ and $T(a, \frac{a+b}{2}) + T(\frac{a+b}{2}, b)$ be the single and double applications of the Trapezoidal rule to $\int_a^b f(x)\,dx$. Derive the relationship between

$$\left|T(a, b) - T\left(a, \frac{a+b}{2}\right) - T\left(\frac{a+b}{2}, b\right)\right|$$

and

$$\left|\int_a^b f(x)\,dx - T\left(a, \frac{a+b}{2}\right) - T\left(\frac{a+b}{2}, b\right)\right|.$$

**10.** The study of light diffraction at a rectangular aperture involves the Fresnel integrals

$$c(t) = \int_0^t \cos \frac{\pi}{2}\omega^2\,d\omega \quad \text{and} \quad s(t) = \int_0^t \sin \frac{\pi}{2}\omega^2\,d\omega.$$

Construct a table of values for $c(t)$ and $s(t)$ that is accurate to within $10^{-4}$ for values of $t = 0.1, 0.2, \ldots, 1.0$.

## 4.7 Gaussian Quadrature

The Newton-Cotes formulas in Section 4.3 were derived by integrating interpolating polynomials. The error term in the interpolating polynomial of degree $n$ involves the $(n + 1)$st derivative of the function being approximated, so a Newton-Cotes formula is exact when approximating the integral of any polynomial of degree less than or equal to $n$.

All the Newton-Cotes formulas use values of the function at equally-spaced points. This restriction is convenient when the formulas are combined to form the composite rules we considered in Section 4.4, but it can significantly decrease the accuracy of the approximation. Consider, for example, the Trapezoidal rule applied to determine the integrals of the functions whose graphs are shown in Figure 4.15.

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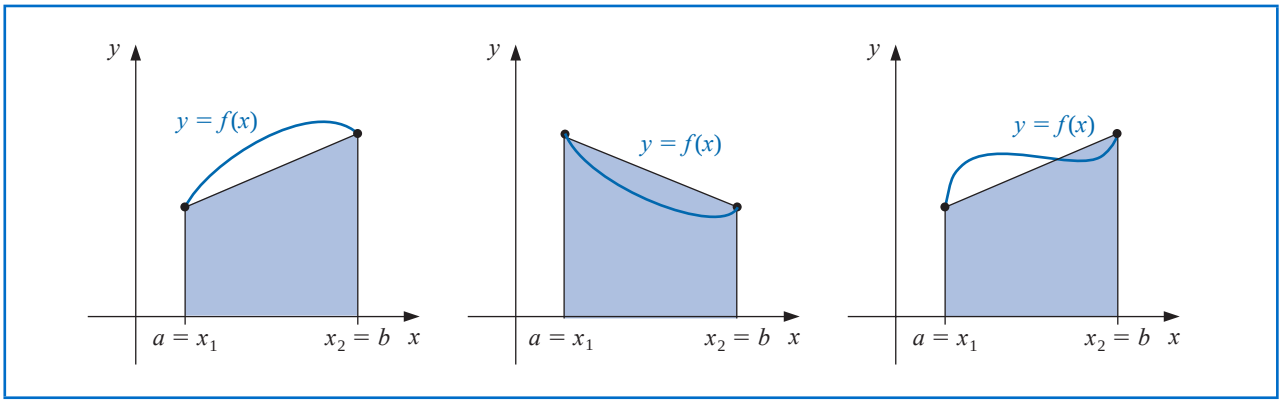
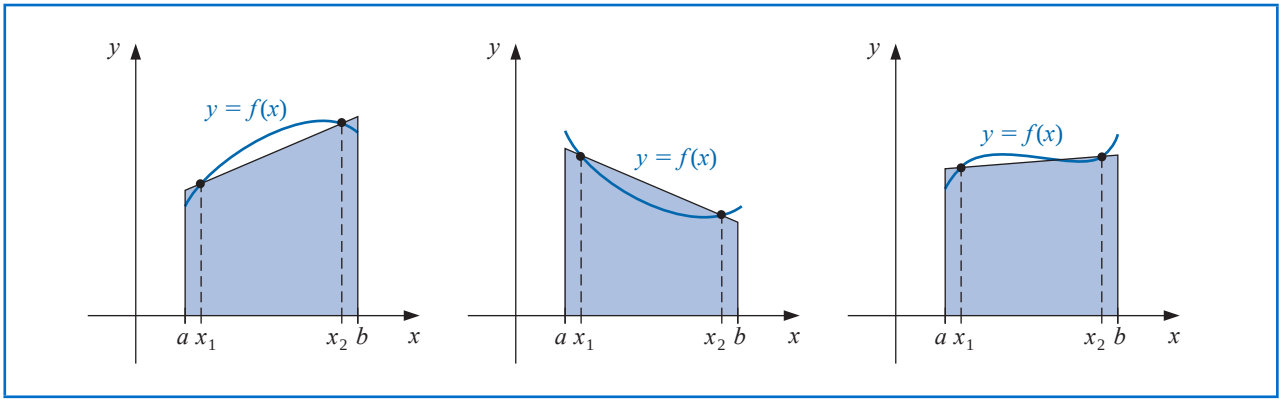
**Figure 4.15**




The Trapezoidal rule approximates the integral of the function by integrating the linear function that joins the endpoints of the graph of the function. But this is not likely the best line for approximating the integral. Lines such as those shown in Figure 4.16 would likely give much better approximations in most cases.

**Figure 4.16**




Gauss demonstrated his method of efficient numerical integration in a paper that was presented to the Göttingen Society in 1814. He let the nodes as well as the coefficients of the function evaluations be parameters in the summation formula and found the optimal placement of the nodes. Goldstine [Golds], pp 224–232, has an interesting description of his development.

Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally-spaced, way. The nodes $x_1, x_2, \ldots, x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, \ldots, c_n$, are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i).$$

To measure this accuracy, we assume that the best choice of these values produces the exact result for the largest class of polynomials, that is, the choice that gives the greatest degree of precision.

The coefficients $c_1, c_2, \ldots, c_n$ in the approximation formula are arbitrary, and the nodes $x_1, x_2, \ldots, x_n$ are restricted only by the fact that they must lie in $[a, b]$, the interval of integration. This gives us $2n$ parameters to choose. If the coefficients of a polynomial are

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considered parameters, the class of polynomials of degree at most $2n - 1$ also contains $2n$ parameters. This, then, is the largest class of polynomials for which it is reasonable to expect a formula to be exact. With the proper choice of the values and constants, exactness on this set can be obtained.

To illustrate the procedure for choosing the appropriate parameters, we will show how to select the coefficients and nodes when $n = 2$ and the interval of integration is $[-1, 1]$. We will then discuss the more general situation for an arbitrary choice of nodes and coefficients and show how the technique is modified when integrating over an arbitrary interval.

Suppose we want to determine $c_1$, $c_2$, $x_1$, and $x_2$ so that the integration formula

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2)$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2(2) - 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3,$$

for some collection of constants, $a_0$, $a_1$, $a_2$, and $a_3$. Because

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\,dx = a_0 \int 1\,dx + a_1 \int x\,dx + a_2 \int x^2\,dx + a_3 \int x^3\,dx,$$

this is equivalent to showing that the formula gives exact results when $f(x)$ is 1, $x$, $x^2$, and $x^3$. Hence, we need $c_1$, $c_2$, $x_1$, and $x_2$, so that

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1\,dx = 2, \qquad c_1 \cdot x_1 + c_2 \cdot x_2 = \int_{-1}^{1} x\,dx = 0,$$

$$c_1 \cdot x_1^2 + c_2 \cdot x_2^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}, \quad \text{and} \quad c_1 \cdot x_1^3 + c_2 \cdot x_2^3 = \int_{-1}^{1} x^3\,dx = 0.$$

A little algebra shows that this system of equations has the unique solution

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3}, \quad \text{and} \quad x_2 = \frac{\sqrt{3}}{3},$$

which gives the approximation formula

$$\int_{-1}^{1} f(x)\,dx \approx f\left(\frac{-\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right). \tag{4.40}$$

This formula has degree of precision 3, that is, it produces the exact result for every polynomial of degree 3 or less.

## Legendre Polynomials

The technique we have described could be used to determine the nodes and coefficients for formulas that give exact results for higher-degree polynomials, but an alternative method obtains them more easily. In Sections 8.2 and 8.3 we will consider various collections of orthogonal polynomials, functions that have the property that a particular definite integral of the product of any two of them is 0. The set that is relevant to our problem is the Legendre polynomials, a collection $\{P_0(x), P_1(x), \ldots, P_n(x), \ldots,\}$ with properties:

**(1)** For each $n$, $P_n(x)$ is a monic polynomial of degree $n$.

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**(2)** $\int_{-1}^{1} P(x)P_n(x)\,dx = 0$ whenever $P(x)$ is a polynomial of degree less than $n$.

Recall that *monic* polynomials have leading coefficient 1.

The first few Legendre polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = x^2 - \frac{1}{3},$$

$$P_3(x) = x^3 - \frac{3}{5}x, \quad \text{and} \quad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}.$$

Adrien-Marie Legendre (1752–1833) introduced this set of polynomials in 1785. He had numerous priority disputes with Gauss, primarily due to Gauss' failure to publish many of his original results until long after he had discovered them.

The roots of these polynomials are distinct, lie in the interval $(-1, 1)$, have a symmetry with respect to the origin, and, most importantly, are the correct choice for determining the parameters that give us the nodes and coefficients for our quadrature method.

The nodes $x_1, x_2, \ldots, x_n$ needed to produce an integral approximation formula that gives exact results for any polynomial of degree less than $2n$ are the roots of the $n$th-degree Legendre polynomial. This is established by the following result.

***Theorem 4.7*** Suppose that $x_1, x_2, \ldots, x_n$ are the roots of the $n$th Legendre polynomial $P_n(x)$ and that for each $i = 1, 2, \ldots, n$, the numbers $c_i$ are defined by

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx.$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x)\,dx = \sum_{i=1}^{n} c_i P(x_i).$$

■

***Proof*** Let us first consider the situation for a polynomial $P(x)$ of degree less than $n$. Rewrite $P(x)$ in terms of $(n-1)$st Lagrange coefficient polynomials with nodes at the roots of the $n$th Legendre polynomial $P_n(x)$. The error term for this representation involves the $n$th derivative of $P(x)$. Since $P(x)$ is of degree less than $n$, the $n$th derivative of $P(x)$ is 0, and this representation of is exact. So

$$P(x) = \sum_{i=1}^{n} P(x_i)L_i(x) = \sum_{i=1}^{n} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i)$$

and

$$\int_{-1}^{1} P(x)\,dx = \int_{-1}^{1} \left[ \sum_{i=1}^{n} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i) \right] dx$$

$$= \sum_{i=1}^{n} \left[ \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\,dx \right] P(x_i) = \sum_{i=1}^{n} c_i P(x_i).$$

Hence the result is true for polynomials of degree less than $n$.

Now consider a polynomial $P(x)$ of degree at least $n$ but less than $2n$. Divide $P(x)$ by the $n$th Legendre polynomial $P_n(x)$. This gives two polynomials $Q(x)$ and $R(x)$, each of degree less than $n$, with

$$P(x) = Q(x)P_n(x) + R(x).$$

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Note that $x_i$ is a root of $P_n(x)$ for each $i = 1, 2, \ldots, n$, so we have

$$P(x_i) = Q(x_i)P_n(x_i) + R(x_i) = R(x_i).$$

We now invoke the unique power of the Legendre polynomials. First, the degree of the polynomial $Q(x)$ is less than $n$, so (by Legendre property **(2)**),

$$\int_{-1}^{1} Q(x)P_n(x)\,dx = 0.$$

Then, since $R(x)$ is a polynomial of degree less than $n$, the opening argument implies that

$$\int_{-1}^{1} R(x)\,dx = \sum_{i=1}^{n} c_i R(x_i).$$

Putting these facts together verifies that the formula is exact for the polynomial $P(x)$:

$$\int_{-1}^{1} P(x)\,dx = \int_{-1}^{1} [Q(x)P_n(x) + R(x)]\,dx = \int_{-1}^{1} R(x)\,dx = \sum_{i=1}^{n} c_i R(x_i) = \sum_{i=1}^{n} c_i P(x_i).$$

■ ■ ■

The constants $c_i$ needed for the quadrature rule can be generated from the equation in Theorem 4.7, but both these constants and the roots of the Legendre polynomials are extensively tabulated. Table 4.12 lists these values for $n = 2, 3, 4$, and 5.

**Table 4.12**

| $n$ | Roots $r_{n,i}$ | Coefficients $c_{n,i}$ |
|---|---|---|
| 2 | 0.5773502692 | 1.0000000000 |
| | −0.5773502692 | 1.0000000000 |
| 3 | 0.7745966692 | 0.5555555556 |
| | 0.0000000000 | 0.8888888889 |
| | −0.7745966692 | 0.5555555556 |
| 4 | 0.8611363116 | 0.3478548451 |
| | 0.3399810436 | 0.6521451549 |
| | −0.3399810436 | 0.6521451549 |
| | −0.8611363116 | 0.3478548451 |
| 5 | 0.9061798459 | 0.2369268850 |
| | 0.5384693101 | 0.4786286705 |
| | 0.0000000000 | 0.5688888889 |
| | −0.5384693101 | 0.4786286705 |
| | −0.9061798459 | 0.2369268850 |

**Example 1** Approximate $\int_{-1}^{1} e^x \cos x\,dx$ using Gaussian quadrature with $n = 3$.

***Solution*** The entries in Table 4.12 give us

$$\begin{aligned}\int_{-1}^{1} e^x \cos x\,dx &\approx 0.\overline{5}e^{0.774596692}\cos 0.774596692 \\ &\quad + 0.\overline{8}\cos 0 + 0.\overline{5}e^{-0.774596692}\cos(-0.774596692) \\ &= 1.9333904.\end{aligned}$$

Integration by parts can be used to show that the true value of the integral is 1.9334214, so the absolute error is less than $3.2 \times 10^{-5}$. ■

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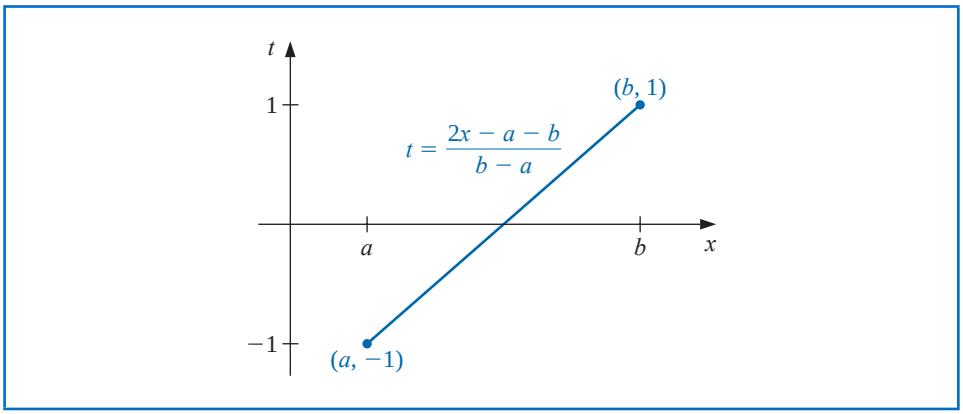
## Gaussian Quadrature on Arbitrary Intervals

An integral $\int_a^b f(x)\,dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables (see Figure 4.17):

$$t = \frac{2x - a - b}{b - a} \iff x = \frac{1}{2}[(b - a)t + a + b].$$

**Figure 4.17**




This permits Gaussian quadrature to be applied to any interval $[a, b]$, because

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b - a)t + (b + a)}{2}\right)\frac{(b - a)}{2}\,dt. \tag{4.41}$$

**Example 2** Consider the integral $\int_1^3 x^6 - x^2 \sin(2x)\,dx = 317.3442466$.

**(a)** Compare the results for the closed Newton-Cotes formula with $n = 1$, the open Newton-Cotes formula with $n = 1$, and Gaussian Quadrature when $n = 2$.

**(b)** Compare the results for the closed Newton-Cotes formula with $n = 2$, the open Newton-Cotes formula with $n = 2$, and Gaussian Quadrature when $n = 3$.

***Solution*** **(a)** Each of the formulas in this part requires 2 evaluations of the function $f(x) = x^6 - x^2 \sin(2x)$. The Newton-Cotes approximations are

$$\textbf{Closed } \boldsymbol{n = 1}: \quad \frac{2}{2}[f(1) + f(3)] = 731.6054420;$$

$$\textbf{Open } \boldsymbol{n = 1}: \quad \frac{3(2/3)}{2}[f(5/3) + f(7/3)] = 188.7856682.$$

Gaussian quadrature applied to this problem requires that the integral first be transformed into a problem whose interval of integration is $[-1, 1]$. Using Eq. (4.41) gives

$$\int_1^3 x^6 - x^2 \sin(2x)\,dx = \int_{-1}^{1} (t + 2)^6 - (t + 2)^2 \sin(2(t + 2))\,dt.$$

Gaussian quadrature with $n = 2$ then gives

$$\int_1^3 x^6 - x^2 \sin(2x)\,dx \approx f(-0.5773502692 + 2) + f(0.5773502692 + 2) = 306.8199344;$$

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**(b)** Each of the formulas in this part requires 3 function evaluations. The Newton-Cotes approximations are

$$\textbf{Closed } n = 2: \quad \frac{(1)}{3}[f(1) + 4f(2) + f(3)] = 333.2380940;$$

$$\textbf{Open } n = 2: \quad \frac{4(1/2)}{3}[2f(1.5) - f(2) + 2f(2.5)] = 303.5912023.$$

Gaussian quadrature with $n = 3$, once the transformation has been done, gives

$$\int_1^3 x^6 - x^2 \sin(2x)\,dx \approx 0.\overline{5}f(-0.7745966692 + 2) + 0.\overline{8}f(2) + 0.\overline{5}f(0.7745966692 + 2) = 317.2641516.$$

The Gaussian quadrature results are clearly superior in each instance. ■

Maple has Composite Gaussian Quadrature in the *NumericalAnalysis* subpackage of Maple's *Student* package. The default for the number of partitions in the command is 10, so the results in Example 2 would be found for $n = 2$ with

$f := x^6 - x^2 \sin(2x); a := 1; b := 3:$
$Quadrature(f(x), x = a..b, method = gaussian[2], partition = 1, output = information)$

which returns the approximation, what Maple assumes is the exact value of the integral, the absolute, and relative errors in the approximations, and the number of function evaluations.

The result when $n = 3$ is, of course, obtained by replacing the statement *method* = *gaussian*[2] with *method* = *gaussian*[3].

## EXERCISE SET 4.7

**1.** Approximate the following integrals using Gaussian quadrature with $n = 2$, and compare your results to the exact values of the integrals.

**a.** $\displaystyle\int_1^{1.5} x^2 \ln x\,dx$

**b.** $\displaystyle\int_0^1 x^2 e^{-x}\,dx$

**c.** $\displaystyle\int_0^{0.35} \frac{2}{x^2 - 4}\,dx$

**d.** $\displaystyle\int_0^{\pi/4} x^2 \sin x\,dx$

**e.** $\displaystyle\int_0^{\pi/4} e^{3x} \sin 2x\,dx$

**f.** $\displaystyle\int_1^{1.6} \frac{2x}{x^2 - 4}\,dx$

**g.** $\displaystyle\int_3^{3.5} \frac{x}{\sqrt{x^2 - 4}}\,dx$

**h.** $\displaystyle\int_0^{\pi/4} (\cos x)^2\,dx$

**2.** Repeat Exercise 1 with $n = 3$.

**3.** Repeat Exercise 1 with $n = 4$.

**4.** Repeat Exercise 1 with $n = 5$.

**5.** Determine constants $a$, $b$, $c$, and $d$ that will produce a quadrature formula

$$\int_{-1}^1 f(x)\,dx = af(-1) + bf(1) + cf'(-1) + df'(1)$$

that has degree of precision 3.

**6.** Determine constants $a$, $b$, $c$, and $d$ that will produce a quadrature formula

$$\int_{-1}^1 f(x)\,dx = af(-1) + bf(0) + cf(1) + df'(-1) + ef'(1)$$

that has degree of precision 4.

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7. Verify the entries for the values of $n = 2$ and 3 in Table 4.12 on page 232 by finding the roots of the respective Legendre polynomials, and use the equations preceding this table to find the coefficients associated with the values.
8. Show that the formula $Q(P) = \sum_{i=1}^{n} c_i P(x_i)$ cannot have degree of precision greater than $2n - 1$, regardless of the choice of $c_1, \ldots, c_n$ and $x_1, \ldots, x_n$. [*Hint:* Construct a polynomial that has a double root at each of the $x_i$'s.]
9. Apply Maple's Composite Gaussian Quadrature routine to approximate $\int_{-1}^{1} x^2 e^x \, dx$ in the following manner.
   **a.** Use Gaussian Quadrature with $n = 8$ on the single interval $[-1, 1]$.
   **b.** Use Gaussian Quadrature with $n = 4$ on the intervals $[-1, 0]$ and $[0, 1]$.
   **c.** Use Gaussian Quadrature with $n = 2$ on the intervals $[-1, -0.5]$, $[-0.5, 0]$, $[0, 0.5]$ and $[0.5, 1]$.
   **d.** Give an explanation for the accuracy of the results.

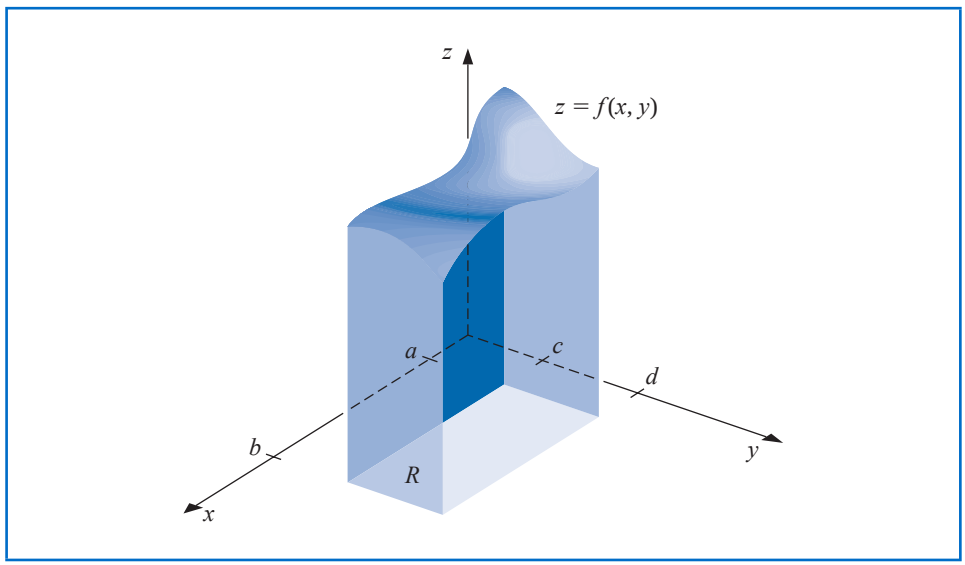
## 4.8 Multiple Integrals

The techniques discussed in the previous sections can be modified for use in the approximation of multiple integrals. Consider the double integral

$$\iint_R f(x, y) \, dA,$$

where $R = \{(x, y) \mid a \le x \le b, c \le y \le d\}$, for some constants $a$, $b$, $c$, and $d$, is a rectangular region in the plane. (See Figure 4.18.)

**Figure 4.18**




The following illustration shows how the Composite Trapezoidal rule using two subintervals in each coordinate direction would be applied to this integral.

**Illustration** Writing the double integral as an iterated integral gives

$$\iint_R f(x, y) \, dA = \int_a^b \left( \int_c^d f(x, y) \, dy \right) dx.$$

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To simplify notation, let $k = (d-c)/2$ and $h = (b-a)/2$. Apply the Composite Trapezoidal rule to the interior integral to obtain

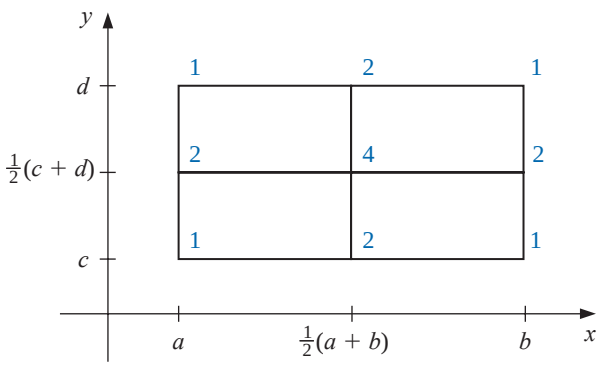
$$\int_c^d f(x,y)\,dy \approx \frac{k}{2}\left[f(x,c) + f(x,d) + 2f\left(x, \frac{c+d}{2}\right)\right].$$

This approximation is of order $O\left((d-c)^3\right)$. Then apply the Composite Trapezoidal rule again to approximate the integral of this function of $x$:

$$\begin{aligned}
\int_a^b \left(\int_c^d f(x,y)\,dy\right) dx &\approx \int_a^b \left(\frac{d-c}{4}\right)\left[f(x,c) + 2f\left(x, \frac{c+d}{2}\right) + f(d)\right] dx \\
&= \frac{b-a}{4}\left(\frac{d-c}{4}\right)\left[f(a,c) + 2f\left(a, \frac{c+d}{2}\right) + f(a,d)\right] \\
&\quad + \frac{b-a}{4}\left(2\left(\frac{d-c}{4}\right)\left[f\left(\frac{a+b}{2}, c\right)\right.\right. \\
&\quad \left.\left. + 2f\left(\frac{a+b}{2}, \frac{c+d}{2}\right) + \left(\frac{a+b}{2}, d\right)\right]\right) \\
&\quad + \frac{b-a}{4}\left(\frac{d-c}{4}\right)\left[f(b,c) + 2f\left(b, \frac{c+d}{2}\right) + f(b,d)\right] \\
&= \frac{(b-a)(d-c)}{16}\left[f(a,c) + f(a,d) + f(b,c) + f(b,d)\right. \\
&\quad + 2\left(f\left(\frac{a+b}{2}, c\right) + f\left(\frac{a+b}{2}, d\right) + f\left(a, \frac{c+d}{2}\right)\right. \\
&\quad \left.\left. + f\left(b, \frac{c+d}{2}\right)\right) + 4f\left(\frac{a+b}{2}, \frac{c+d}{2}\right)\right]
\end{aligned}$$

This approximation is of order $O\left((b-a)(d-c)\left[(b-a)^2 + (d-c)^2\right]\right)$. Figure 4.19 shows a grid with the number of functional evaluations at each of the nodes used in the approximation. □

**Figure 4.19**

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As the illustration shows, the procedure is quite straightforward. But the number of function evaluations grows with the square of the number required for a single integral. In a practical situation we would not expect to use a method as elementary as the Composite Trapezoidal rule. Instead we will employ the Composite Simpson's rule to illustrate the general approximation technique, although any other composite formula could be used in its place.

To apply the Composite Simpson's rule, we divide the region $R$ by partitioning both $[a, b]$ and $[c, d]$ into an even number of subintervals. To simplify the notation, we choose even integers $n$ and $m$ and partition $[a, b]$ and $[c, d]$ with the evenly spaced mesh points $x_0, x_1, \ldots, x_n$ and $y_0, y_1, \ldots, y_m$, respectively. These subdivisions determine step sizes $h = (b - a)/n$ and $k = (d - c)/m$. Writing the double integral as the iterated integral

$$\iint_R f(x, y)\, dA = \int_a^b \left( \int_c^d f(x, y)\, dy \right) dx,$$

we first use the Composite Simpson's rule to approximate

$$\int_c^d f(x, y)\, dy,$$

treating $x$ as a constant.

Let $y_j = c + jk$, for each $j = 0, 1, \ldots, m$. Then

$$\int_c^d f(x, y)\, dy = \frac{k}{3}\left[ f(x, y_0) + 2 \sum_{j=1}^{(m/2)-1} f(x, y_{2j}) + 4 \sum_{j=1}^{m/2} f(x, y_{2j-1}) + f(x, y_m) \right] - \frac{(d - c)k^4}{180} \frac{\partial^4 f}{\partial y^4}(x, \mu),$$

for some $\mu$ in $(c, d)$. Thus

$$\begin{aligned} \int_a^b \int_c^d f(x, y)\, dy\, dx = \frac{k}{3}\Bigg[ & \int_a^b f(x, y_0)\, dx + 2 \sum_{j=1}^{(m/2)-1} \int_a^b f(x, y_{2j})\, dx \\ & + 4 \sum_{j=1}^{m/2} \int_a^b f(x, y_{2j-1})\, dx + \int_a^b f(x, y_m)\, dx \Bigg] \\ & - \frac{(d - c)k^4}{180} \int_a^b \frac{\partial^4 f}{\partial y^4}(x, \mu)\, dx. \end{aligned}$$

Composite Simpson's rule is now employed on the integrals in this equation. Let $x_i = a + ih$, for each $i = 0, 1, \ldots, n$. Then for each $j = 0, 1, \ldots, m$, we have

$$\int_a^b f(x, y_j)\, dx = \frac{h}{3}\left[ f(x_0, y_j) + 2 \sum_{i=1}^{(n/2)-1} f(x_{2i}, y_j) + 4 \sum_{i=1}^{n/2} f(x_{2i-1}, y_j) + f(x_n, y_j) \right] - \frac{(b - a)h^4}{180} \frac{\partial^4 f}{\partial x^4}(\xi_j, y_j),$$

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for some $\xi_j$ in $(a, b)$. The resulting approximation has the form

$$\begin{aligned}\int_a^b \int_c^d f(x,y)\,dy\,dx \approx \frac{hk}{9}\Bigg\{&\Bigg[f(x_0,y_0)+2\sum_{i=1}^{(n/2)-1} f(x_{2i},y_0)\\&+4\sum_{i=1}^{n/2} f(x_{2i-1},y_0)+f(x_n,y_0)\Bigg]\\&+2\Bigg[\sum_{j=1}^{(m/2)-1} f(x_0,y_{2j})+2\sum_{j=1}^{(m/2)-1}\sum_{i=1}^{(n/2)-1} f(x_{2i},y_{2j})\\&+4\sum_{j=1}^{(m/2)-1}\sum_{i=1}^{n/2} f(x_{2i-1},y_{2j})+\sum_{j=1}^{(m/2)-1} f(x_n,y_{2j})\Bigg]\\&+4\Bigg[\sum_{j=1}^{m/2} f(x_0,y_{2j-1})+2\sum_{j=1}^{m/2}\sum_{i=1}^{(n/2)-1} f(x_{2i},y_{2j-1})\\&+4\sum_{j=1}^{m/2}\sum_{i=1}^{n/2} f(x_{2i-1},y_{2j-1})+\sum_{j=1}^{m/2} f(x_n,y_{2j-1})\Bigg]\\&+\Bigg[f(x_0,y_m)+2\sum_{i=1}^{(n/2)-1} f(x_{2i},y_m)+4\sum_{i=1}^{n/2} f(x_{2i-1},y_m)+f(x_n,y_m)\Bigg]\Bigg\}.\end{aligned}$$

The error term $E$ is given by

$$\begin{aligned}E=\frac{-k(b-a)h^4}{540}\Bigg[&\frac{\partial^4 f}{\partial x^4}(\xi_0,y_0)+2\sum_{j=1}^{(m/2)-1}\frac{\partial^4 f}{\partial x^4}(\xi_{2j},y_{2j})+4\sum_{j=1}^{m/2}\frac{\partial^4 f}{\partial x^4}(\xi_{2j-1},y_{2j-1})\\&+\frac{\partial^4 f}{\partial x^4}(\xi_m,y_m)\Bigg]-\frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f}{\partial y^4}(x,\mu)\,dx.\end{aligned}$$

If $\partial^4 f/\partial x^4$ is continuous, the Intermediate Value Theorem 1.11 can be repeatedly applied to show that the evaluation of the partial derivatives with respect to $x$ can be replaced by a common value and that

$$E=\frac{-k(b-a)h^4}{540}\left[3m\frac{\partial^4 f}{\partial x^4}(\overline{\eta},\overline{\mu})\right]-\frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f}{\partial y^4}(x,\mu)\,dx,$$

for some $(\overline{\eta}, \overline{\mu})$ in $R$. If $\partial^4 f/\partial y^4$ is also continuous, the Weighted Mean Value Theorem for Integrals 1.13 implies that

$$\int_a^b \frac{\partial^4 f}{\partial y^4}(x,\mu)\,dx=(b-a)\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu}),$$

for some $(\hat{\eta}, \hat{\mu})$ in $R$. Because $m = (d - c)/k$, the error term has the form

$$E=\frac{-k(b-a)h^4}{540}\left[3m\frac{\partial^4 f}{\partial x^4}(\overline{\eta},\overline{\mu})\right]-\frac{(d-c)(b-a)}{180}k^4\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu})$$

which simplifies to

$$E=-\frac{(d-c)(b-a)}{180}\left[h^4\frac{\partial^4 f}{\partial x^4}(\overline{\eta},\overline{\mu})+k^4\frac{\partial^4 f}{\partial y^4}(\hat{\eta},\hat{\mu})\right],$$

for some $(\overline{\eta}, \overline{\mu})$ and $(\hat{\eta}, \hat{\mu})$ in $R$.

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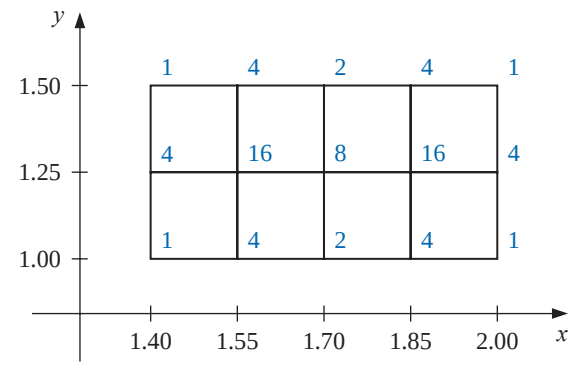
**Example 1** Use Composite Simpson's rule with $n = 4$ and $m = 2$ to approximate

$$\int_{1.4}^{2.0} \int_{1.0}^{1.5} \ln(x + 2y)\, dy\, dx,$$

***Solution*** The step sizes for this application are $h = (2.0 - 1.4)/4 = 0.15$ and $k = (1.5 - 1.0)/2 = 0.25$. The region of integration $R$ is shown in Figure 4.20, together with the nodes $(x_i, y_j)$, where $i = 0, 1, 2, 3, 4$ and $j = 0, 1, 2$. It also shows the coefficients $w_{i,j}$ of $f(x_i, y_i) = \ln(x_i + 2y_i)$ in the sum that gives the Composite Simpson's rule approximation to the integral.

**Figure 4.20**




The approximation is

$$\int_{1.4}^{2.0} \int_{1.0}^{1.5} \ln(x + 2y)\, dy\, dx \approx \frac{(0.15)(0.25)}{9} \sum_{i=0}^{4} \sum_{j=0}^{2} w_{i,j} \ln(x_i + 2y_j)$$

$$= 0.4295524387.$$

We have

$$\frac{\partial^4 f}{\partial x^4}(x, y) = \frac{-6}{(x + 2y)^4} \quad \text{and} \quad \frac{\partial^4 f}{\partial y^4}(x, y) = \frac{-96}{(x + 2y)^4},$$

and the maximum values of the absolute values of these partial derivatives occur on $R$ when $x = 1.4$ and $y = 1.0$. So the error is bounded by

$$|E| \le \frac{(0.5)(0.6)}{180} \left[ (0.15)^4 \max_{(x,y) \text{in} R} \frac{6}{(x + 2y)^4} + (0.25)^4 \max_{(x,y) \text{in} R} \frac{96}{(x + 2y)^4} \right] \le 4.72 \times 10^{-6}.$$

The actual value of the integral to ten decimal places is

$$\int_{1.4}^{2.0} \int_{1.0}^{1.5} \ln(x + 2y)\, dy\, dx = 0.4295545265,$$

so the approximation is accurate to within $2.1 \times 10^{-6}$. ■

The same techniques can be applied for the approximation of triple integrals as well as higher integrals for functions of more than three variables. The number of functional evaluations required for the approximation is the product of the number of functional evaluations required when the method is applied to each variable.

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## Gaussian Quadrature for Double Integral Approximation

To reduce the number of functional evaluations, more efficient methods such as Gaussian quadrature, Romberg integration, or Adaptive quadrature can be incorporated in place of the Newton-Cotes formulas. The following example illustrates the use of Gaussian quadrature for the integral considered in Example 1.

**Example 2** Use Gaussian quadrature with $n = 3$ in both dimensions to approximate the integral

$$\int_{1.4}^{2.0} \int_{1.0}^{1.5} \ln(x + 2y)\, dy\, dx.$$

***Solution*** Before employing Gaussian quadrature to approximate this integral, we need to transform the region of integration

$$R = \{ (x, y) \mid 1.4 \le x \le 2.0, 1.0 \le y \le 1.5 \}$$

into

$$\hat{R} = \{ (u, v) \mid -1 \le u \le 1, -1 \le v \le 1 \}.$$

The linear transformations that accomplish this are

$$u = \frac{1}{2.0 - 1.4}(2x - 1.4 - 2.0) \quad \text{and} \quad v = \frac{1}{1.5 - 1.0}(2y - 1.0 - 1.5),$$

or, equivalently, $x = 0.3u + 1.7$ and $y = 0.25v + 1.25$. Employing this change of variables gives an integral on which Gaussian quadrature can be applied:

$$\int_{1.4}^{2.0} \int_{1.0}^{1.5} \ln(x + 2y)\, dy\, dx = 0.075 \int_{-1}^{1} \int_{-1}^{1} \ln(0.3u + 0.5v + 4.2)\, dv\, du.$$

The Gaussian quadrature formula for $n = 3$ in both $u$ and $v$ requires that we use the nodes

$$u_1 = v_1 = r_{3,2} = 0, \quad u_0 = v_0 = r_{3,1} = -0.7745966692,$$

and

$$u_2 = v_2 = r_{3,3} = 0.7745966692.$$

The associated weights are $c_{3,2} = 0.\overline{8}$ and $c_{3,1} = c_{3,3} = 0.\overline{5}$. (These are given in Table 4.12 on page 232.) The resulting approximation is

$$\int_{1.4}^{2.0} \int_{1.0}^{1.5} \ln(x + 2y)\, dy\, dx \approx 0.075 \sum_{i=1}^{3} \sum_{j=1}^{3} c_{3,i} c_{3,j} \ln(0.3r_{3,i} + 0.5r_{3,j} + 4.2)$$

$$= 0.4295545313.$$

Although this result requires only 9 functional evaluations compared to 15 for the Composite Simpson's rule considered in Example 1, it is accurate to within $4.8 \times 10^{-9}$, compared to $2.1 \times 10^{-6}$ accuracy in Example 1. ■

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## Non-Rectangular Regions

The use of approximation methods for double integrals is not limited to integrals with rectangular regions of integration. The techniques previously discussed can be modified to approximate double integrals of the form

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y)\, dy\, dx \tag{4.42}$$

or

$$\int_c^d \int_{a(y)}^{b(y)} f(x, y)\, dx\, dy. \tag{4.43}$$

In fact, integrals on regions not of this type can also be approximated by performing appropriate partitions of the region. (See Exercise 10.)

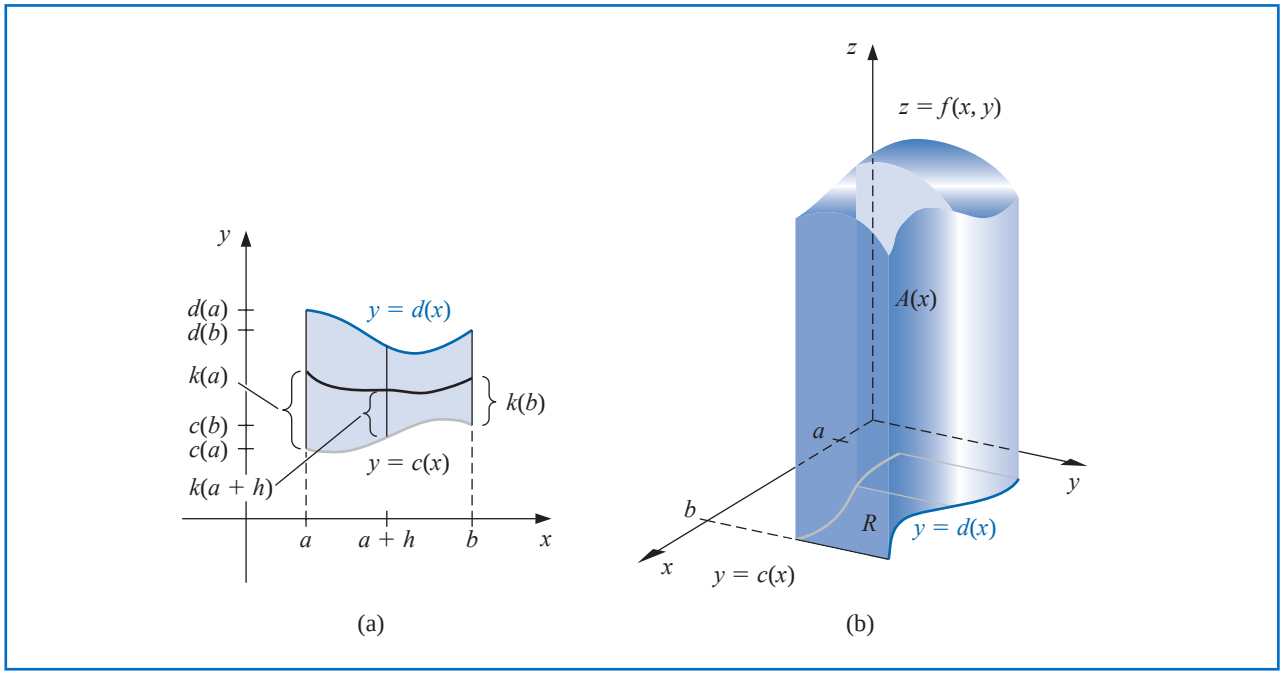
To describe the technique involved with approximating an integral in the form

$$\int_a^b \int_{c(x)}^{d(x)} f(x, y)\, dy\, dx,$$

we will use the basic Simpson's rule to integrate with respect to both variables. The step size for the variable $x$ is $h = (b - a)/2$, but the step size for $y$ varies with $x$ (see Figure 4.21) and is written

$$k(x) = \frac{d(x) - c(x)}{2}.$$

**Figure 4.21**

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This gives

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx \approx \int_a^b \frac{k(x)}{3}[f(x,c(x)) + 4f(x,c(x)+k(x)) + f(x,d(x))]\,dx$$

$$\approx \frac{h}{3}\left\{\frac{k(a)}{3}[f(a,c(a)) + 4f(a,c(a)+k(a)) + f(a,d(a))]\right.$$

$$+ \frac{4k(a+h)}{3}[f(a+h,c(a+h)) + 4f(a+h,c(a+h)$$

$$+ k(a+h)) + f(a+h,d(a+h))]$$

$$\left. + \frac{k(b)}{3}[f(b,c(b)) + 4f(b,c(b)+k(b)) + f(b,d(b))]\right\}.$$

Algorithm 4.4 applies the Composite Simpson's rule to an integral in the form (4.42). Integrals in the form (4.43) can, of course, be handled similarly.

ALGORITHM
**4.4**

## Simpson's Double Integral

To approximate the integral

$$I = \int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx:$$

INPUT endpoints $a, b$: even positive integers $m, n$.

OUTPUT approximation $J$ to $I$.

*Step 1* Set $h = (b-a)/n$;
$J_1 = 0$; (*End terms.*)
$J_2 = 0$; (*Even terms.*)
$J_3 = 0$. (*Odd terms.*)

*Step 2* For $i = 0, 1, \ldots, n$ do Steps 3–8.

*Step 3* Set $x = a + ih$; (*Composite Simpson's method for x.*)
$HX = (d(x) - c(x))/m$;
$K_1 = f(x,c(x)) + f(x,d(x))$; (*End terms.*)
$K_2 = 0$; (*Even terms.*)
$K_3 = 0$. (*Odd terms.*)

*Step 4* For $j = 1, 2, \ldots, m-1$ do Step 5 and 6.

*Step 5* Set $y = c(x) + jHX$;
$Q = f(x,y)$.

*Step 6* If $j$ is even then set $K_2 = K_2 + Q$
else set $K_3 = K_3 + Q$.

*Step 7* Set $L = (K_1 + 2K_2 + 4K_3)HX/3$.

$\left(L \approx \int_{c(x_i)}^{d(x_i)} f(x_i,y)\,dy \quad \textit{by the Composite Simpson's method.}\right)$

*Step 8* If $i = 0$ or $i = n$ then set $J_1 = J_1 + L$
else if $i$ is even then set $J_2 = J_2 + L$
else set $J_3 = J_3 + L$.

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*Step 9* Set $J = h(J_1 + 2J_2 + 4J_3)/3$.

*Step 10* OUTPUT $(J)$;
STOP. ■

To apply Gaussian quadrature to the double integral

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx,$$

first requires transforming, for each $x$ in $[a,b]$, the variable $y$ in the interval $[c(x),d(x)]$ into the variable $t$ in the interval $[-1,1]$. This linear transformation gives

$$f(x,y) = f\left(x, \frac{(d(x)-c(x))t + d(x) + c(x)}{2}\right) \quad \text{and} \quad dy = \frac{d(x)-c(x)}{2}\,dt.$$

The reduced calculation makes it generally worthwhile to apply Gaussian quadrature rather than a Simpson's technique when approximating double integrals.

Then, for each $x$ in $[a,b]$, we apply Gaussian quadrature to the resulting integral

$$\int_{c(x)}^{d(x)} f(x,y)\,dy = \int_{-1}^{1} f\left(x, \frac{(d(x)-c(x))t + d(x) + c(x)}{2}\right) dt$$

to produce

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx \approx \int_a^b \frac{d(x)-c(x)}{2} \sum_{j=1}^{n} c_{n,j} f\left(x, \frac{(d(x)-c(x))r_{n,j} + d(x) + c(x)}{2}\right) dx,$$

where, as before, the roots $r_{n,j}$ and coefficients $c_{n,j}$ come from Table 4.12 on page 232. Now the interval $[a,b]$ is transformed to $[-1,1]$, and Gaussian quadrature is applied to approximate the integral on the right side of this equation. The details are given in Algorithm 4.5.

ALGORITHM
**4.5**

## Gaussian Double Integral

To approximate the integral

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx :$$

INPUT endpoints $a, b$; positive integers $m, n$.
(*The roots $r_{i,j}$ and coefficients $c_{i,j}$ need to be available for $i = \max\{m,n\}$ and for $1 \le j \le i$.*)

OUTPUT approximation $J$ to $I$.

*Step 1* Set $h_1 = (b-a)/2$;
$h_2 = (b+a)/2$;
$J = 0$.

*Step 2* For $i = 1, 2, \ldots, m$ do Steps 3–5.

*Step 3* Set $JX = 0$;
$x = h_1 r_{m,i} + h_2$;
$d_1 = d(x)$;
$c_1 = c(x)$;
$k_1 = (d_1 - c_1)/2$;
$k_2 = (d_1 + c_1)/2$.

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*Step 4* For $j = 1, 2, \ldots, n$ do
set $y = k_1 r_{n,j} + k_2$;
$Q = f(x, y)$;
$JX = JX + c_{n,j} Q$.

*Step 5* Set $J = J + c_{m,i} k_1 JX$.

*Step 6* Set $J = h_1 J$.

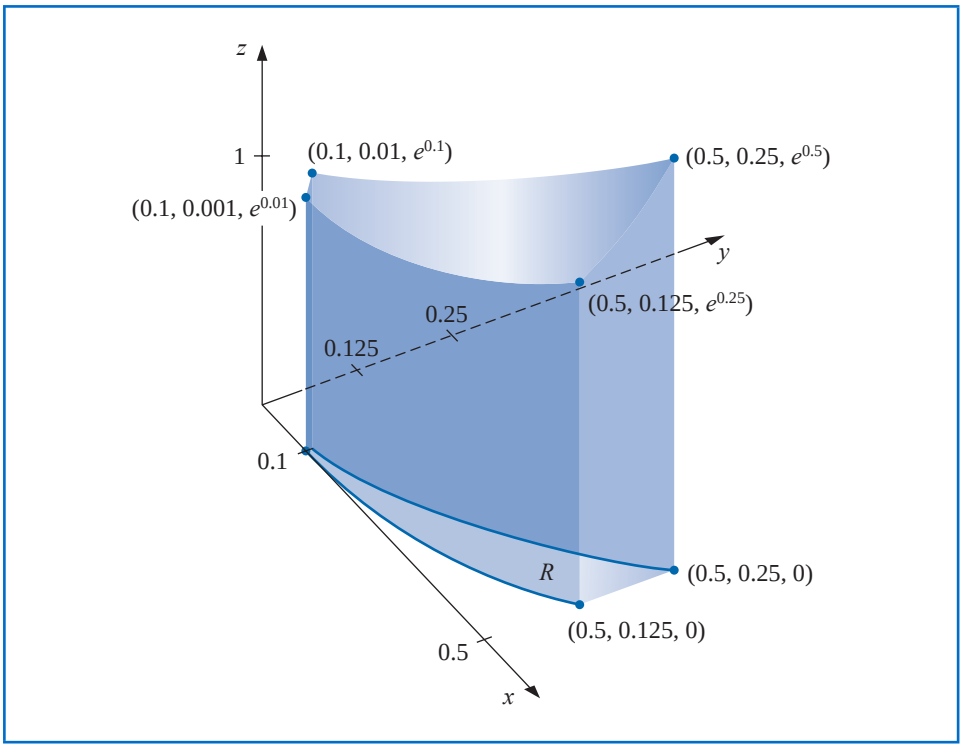
*Step 7* OUTPUT ($J$);
STOP. ■

**Illustration** The volume of the solid in Figure 4.22 is approximated by applying Simpson's Double Integral Algorithm with $n = m = 10$ to

$$\int_{0.1}^{0.5} \int_{x^3}^{x^2} e^{y/x}\, dy\, dx.$$

This requires 121 evaluations of the function $f(x, y) = e^{y/x}$ and produces the value 0.0333054, which approximates the volume of the solid shown in Figure 4.22 to nearly seven decimal places. Applying the Gaussian Quadrature Algorithm with $n = m = 5$ requires only 25 function evaluations and gives the approximation 0.03330556611, which is accurate to 11 decimal places. □

**Figure 4.22**

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## Triple Integral Approximation

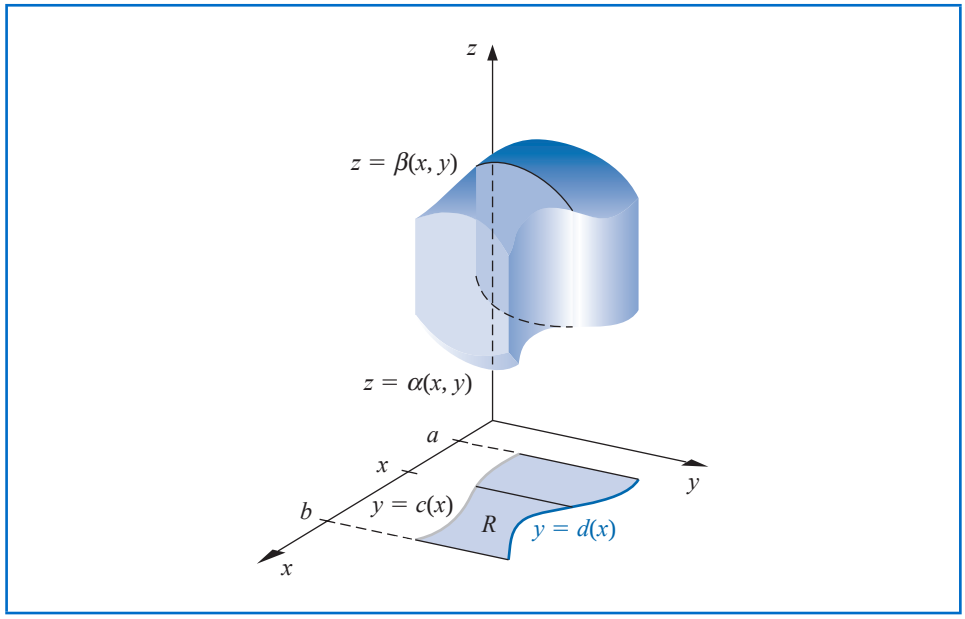
Triple integrals of the form

$$\int_a^b \int_{c(x)}^{d(x)} \int_{\alpha(x,y)}^{\beta(x,y)} f(x, y, z)\, dz\, dy\, dx$$

(see Figure 4.23) are approximated in a similar manner. Because of the number of calculations involved, Gaussian quadrature is the method of choice. Algorithm 4.6 implements this procedure.

The reduced calculation makes it almost always worthwhile to apply Gaussian quadrature rather than a Simpson's technique when approximating triple or higher integrals.

**Figure 4.23**




ALGORITHM
**4.6**

## Gaussian Triple Integral

To approximate the integral

$$\int_a^b \int_{c(x)}^{d(x)} \int_{\alpha(x,y)}^{\beta(x,y)} f(x, y, z)\, dz\, dy\, dx :$$

INPUT endpoints $a, b$; positive integers $m, n, p$.
(*The roots* $r_{i,j}$ *and coefficients* $c_{i,j}$ *need to be available for* $i = \max\{n, m, p\}$ *and for* $1 \le j \le i$.)

OUTPUT approximation $J$ to $I$.

*Step 1* Set $h_1 = (b - a)/2$;
$h_2 = (b + a)/2$;
$J = 0$.

*Step 2* For $i = 1, 2, \ldots, m$ do Steps 3–8.

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*Step 3* Set $JX = 0$;
$x = h_1 r_{m,i} + h_2$;
$d_1 = d(x)$;
$c_1 = c(x)$;
$k_1 = (d_1 - c_1)/2$;
$k_2 = (d_1 + c_1)/2$.

*Step 4* For $j = 1, 2, \ldots, n$ do Steps 5–7.

*Step 5* Set $JY = 0$;
$y = k_1 r_{n,j} + k_2$;
$\beta_1 = \beta(x, y)$;
$\alpha_1 = \alpha(x, y)$;
$l_1 = (\beta_1 - \alpha_1)/2$;
$l_2 = (\beta_1 + \alpha_1)/2$.

*Step 6* For $k = 1, 2, \ldots, p$ do
set $z = l_1 r_{p,k} + l_2$;
$Q = f(x, y, z)$;
$JY = JY + c_{p,k} Q$.

*Step 7* Set $JX = JX + c_{n,j} l_1 JY$.

*Step 8* Set $J = J + c_{m,i} k_1 JX$.

*Step 9* Set $J = h_1 J$.

*Step 10* OUTPUT $(J)$;
STOP. ■

The following example requires the evaluation of four triple integrals.

**Illustration** The center of a mass of a solid region $D$ with density function $\sigma$ occurs at

$$(\bar{x}, \bar{y}, \bar{z}) = \left( \frac{M_{yz}}{M}, \frac{M_{xz}}{M}, \frac{M_{xy}}{M} \right),$$

where

$$M_{yz} = \iiint_D x\sigma(x, y, z)\, dV, \quad M_{xz} = \iiint_D y\sigma(x, y, z)\, dV$$

and

$$M_{xy} = \iiint_D z\sigma(x, y, z)\, dV$$

are the moments about the coordinate planes and the mass of $D$ is

$$M = \iiint_D \sigma(x, y, z)\, dV.$$

The solid shown in Figure 4.24 is bounded by the upper nappe of the cone $z^2 = x^2 + y^2$ and the plane $z = 2$. Suppose that this solid has density function given by

$$\sigma(x, y, z) = \sqrt{x^2 + y^2}.$$

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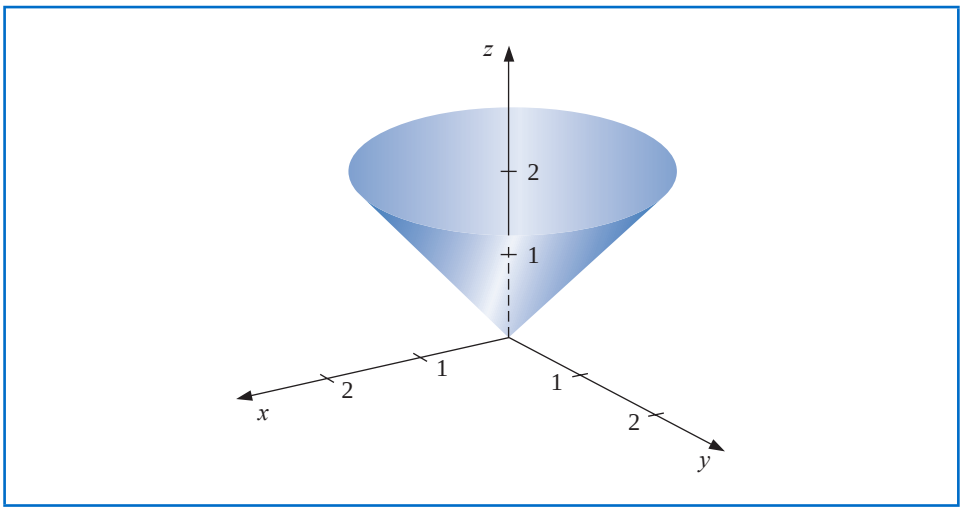
**Figure 4.24**




Applying the Gaussian Triple Integral Algorithm 4.6 with $n = m = p = 5$ requires 125 function evaluations per integral and gives the following approximations:

$$M = \int_{-2}^{2} \int_{-\sqrt{4-x^2}}^{\sqrt{4-x^2}} \int_{\sqrt{x^2+y^2}}^{2} \sqrt{x^2+y^2}\, dz\, dy\, dx$$

$$= 4 \int_{0}^{2} \int_{0}^{\sqrt{4-x^2}} \int_{\sqrt{x^2+y^2}}^{2} \sqrt{x^2+y^2}\, dz\, dy\, dx \approx 8.37504476,$$

$$M_{yz} = \int_{-2}^{2} \int_{-\sqrt{4-x^2}}^{\sqrt{4-x^2}} \int_{\sqrt{x^2+y^2}}^{2} x\sqrt{x^2+y^2}\, dz\, dy\, dx \approx -5.55111512 \times 10^{-17},$$

$$M_{xz} = \int_{-2}^{2} \int_{-\sqrt{4-x^2}}^{\sqrt{4-x^2}} \int_{\sqrt{x^2+y^2}}^{2} y\sqrt{x^2+y^2}\, dz\, dy\, dx \approx -8.01513675 \times 10^{-17},$$

$$M_{xy} = \int_{-2}^{2} \int_{-\sqrt{4-x^2}}^{\sqrt{4-x^2}} \int_{\sqrt{x^2+y^2}}^{2} z\sqrt{x^2+y^2}\, dz\, dy\, dx \approx 13.40038156.$$

This implies that the approximate location of the center of mass is

$$(\bar{x}, \bar{y}, \bar{z}) = (0, 0, 1.60003701).$$

These integrals are quite easy to evaluate directly. If you do this, you will find that the exact center of mass occurs at $(0, 0, 1.6)$. □

Multiple integrals can be evaluated in Maple using the *MultInt* command in the *MultivariateCalculus* subpackage of the *Student* package. For example, to evaluate the multiple integral

$$\int_{2}^{4} \int_{x-1}^{x+6} \int_{-2}^{4+y^2} x^2 + y^2 + z\, dz\, dy\, dx$$

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we first load the package and define the function with

*with*(*Student*[*MultivariateCalculus*]): $f := (x, y, z) \to x^2 + y^2 + z$

Then issue the command

*MultiInt*($f(x, y, z), z = -2..4 + y^2,\ y = x - 1..x + 6,\ x = 2..4$)

which produces the result

1.995885970

## EXERCISE SET 4.8

**1.** Use Algorithm 4.4 with $n = m = 4$ to approximate the following double integrals, and compare the results to the exact answers.

**a.** $\int_{2.1}^{2.5} \int_{1.2}^{1.4} xy^2 \, dy \, dx$

**b.** $\int_{0}^{0.5} \int_{0}^{0.5} e^{y-x} \, dy \, dx$

**c.** $\int_{2}^{2.2} \int_{x}^{2x} (x^2 + y^3) \, dy \, dx$

**d.** $\int_{1}^{1.5} \int_{0}^{x} (x^2 + \sqrt{y}) \, dy \, dx$

**2.** Find the smallest values for $n = m$ so that Algorithm 4.4 can be used to approximate the integrals in Exercise 1 to within $10^{-6}$ of the actual value.

**3.** Use Algorithm 4.4 with (i) $n = 4, m = 8$, (ii) $n = 8, m = 4$, and (iii) $n = m = 6$ to approximate the following double integrals, and compare the results to the exact answers.

**a.** $\int_{0}^{\pi/4} \int_{\sin x}^{\cos x} (2y \sin x + \cos^2 x) \, dy \, dx$

**b.** $\int_{1}^{e} \int_{1}^{x} \ln xy \, dy \, dx$

**c.** $\int_{0}^{1} \int_{x}^{2x} (x^2 + y^3) \, dy \, dx$

**d.** $\int_{0}^{1} \int_{x}^{2x} (y^2 + x^3) \, dy \, dx$

**e.** $\int_{0}^{\pi} \int_{0}^{x} \cos x \, dy \, dx$

**f.** $\int_{0}^{\pi} \int_{0}^{x} \cos y \, dy \, dx$

**g.** $\int_{0}^{\pi/4} \int_{0}^{\sin x} \frac{1}{\sqrt{1 - y^2}} \, dy \, dx$

**h.** $\int_{-\pi}^{3\pi/2} \int_{0}^{2\pi} (y \sin x + x \cos y) \, dy \, dx$

**4.** Find the smallest values for $n = m$ so that Algorithm 4.4 can be used to approximate the integrals in Exercise 3 to within $10^{-6}$ of the actual value.

**5.** Use Algorithm 4.5 with $n = m = 2$ to approximate the integrals in Exercise 1, and compare the results to those obtained in Exercise 1.

**6.** Find the smallest values of $n = m$ so that Algorithm 4.5 can be used to approximate the integrals in Exercise 1 to within $10^{-6}$. Do not continue beyond $n = m = 5$. Compare the number of functional evaluations required to the number required in Exercise 2.

**7.** Use Algorithm 4.5 with (i) $n = m = 3$, (ii) $n = 3, m = 4$, (iii) $n = 4, m = 3$, and (iv) $n = m = 4$ to approximate the integrals in Exercise 3.

**8.** Use Algorithm 4.5 with $n = m = 5$ to approximate the integrals in Exercise 3. Compare the number of functional evaluations required to the number required in Exercise 4.

**9.** Use Algorithm 4.4 with $n = m = 14$ and Algorithm 4.5 with $n = m = 4$ to approximate

$$\iint_R e^{-(x+y)} \, dA,$$

for the region $R$ in the plane bounded by the curves $y = x^2$ and $y = \sqrt{x}$.

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**10.** Use Algorithm 4.4 to approximate

$$\iint_R \sqrt{xy + y^2}\, dA,$$

where $R$ is the region in the plane bounded by the lines $x + y = 6$, $3y - x = 2$, and $3x - y = 2$. First partition $R$ into two regions $R_1$ and $R_2$ on which Algorithm 4.4 can be applied. Use $n = m = 6$ on both $R_1$ and $R_2$.

**11.** A plane lamina is a thin sheet of continuously distributed mass. If $\sigma$ is a function describing the density of a lamina having the shape of a region $R$ in the $xy$-plane, then the center of the mass of the lamina $(\bar{x}, \bar{y})$ is

$$\bar{x} = \frac{\iint_R x\sigma(x, y)\, dA}{\iint_R \sigma(x, y)\, dA}, \quad \bar{y} = \frac{\iint_R y\sigma(x, y)\, dA}{\iint_R \sigma(x, y)\, dA}.$$

Use Algorithm 4.4 with $n = m = 14$ to find the center of mass of the lamina described by $R = \{(x, y) \mid 0 \le x \le 1, 0 \le y \le \sqrt{1 - x^2}\}$ with the density function $\sigma(x, y) = e^{-(x^2+y^2)}$. Compare the approximation to the exact result.

**12.** Repeat Exercise 11 using Algorithm 4.5 with $n = m = 5$.

**13.** The area of the surface described by $z = f(x, y)$ for $(x, y)$ in $R$ is given by

$$\iint_R \sqrt{[f_x(x, y)]^2 + [f_y(x, y)]^2 + 1}\, dA.$$

Use Algorithm 4.4 with $n = m = 8$ to find an approximation to the area of the surface on the hemisphere $x^2 + y^2 + z^2 = 9, z \ge 0$ that lies above the region in the plane described by $R = \{(x, y) \mid 0 \le x \le 1, 0 \le y \le 1\}$.

**14.** Repeat Exercise 13 using Algorithm 4.5 with $n = m = 4$.

**15.** Use Algorithm 4.6 with $n = m = p = 2$ to approximate the following triple integrals, and compare the results to the exact answers.

**a.** $\displaystyle\int_0^1 \int_1^2 \int_0^{0.5} e^{x+y+z}\, dz\, dy\, dx$

**b.** $\displaystyle\int_0^1 \int_x^1 \int_0^y y^2 z\, dz\, dy\, dx$

**c.** $\displaystyle\int_0^1 \int_{x^2}^x \int_{x-y}^{x+y} y\, dz\, dy\, dx$

**d.** $\displaystyle\int_0^1 \int_{x^2}^x \int_{x-y}^{x+y} z\, dz\, dy\, dx$

**e.** $\displaystyle\int_0^\pi \int_0^x \int_0^{xy} \frac{1}{y} \sin\frac{z}{y}\, dz\, dy\, dx$

**f.** $\displaystyle\int_0^1 \int_0^1 \int_{-xy}^{xy} e^{x^2+y^2}\, dz\, dy\, dx$

**16.** Repeat Exercise 15 using $n = m = p = 3$.

**17.** Repeat Exercise 15 using $n = m = p = 4$ and $n = m = p = 5$.

**18.** Use Algorithm 4.6 with $n = m = p = 4$ to approximate

$$\iiint_S xy \sin(yz)\, dV,$$

where $S$ is the solid bounded by the coordinate planes and the planes $x = \pi$, $y = \pi/2$, $z = \pi/3$. Compare this approximation to the exact result.

**19.** Use Algorithm 4.6 with $n = m = p = 5$ to approximate

$$\iiint_S \sqrt{xyz}\, dV,$$

where $S$ is the region in the first octant bounded by the cylinder $x^2 + y^2 = 4$, the sphere $x^2 + y^2 + z^2 = 4$, and the plane $x + y + z = 8$. How many functional evaluations are required for the approximation?

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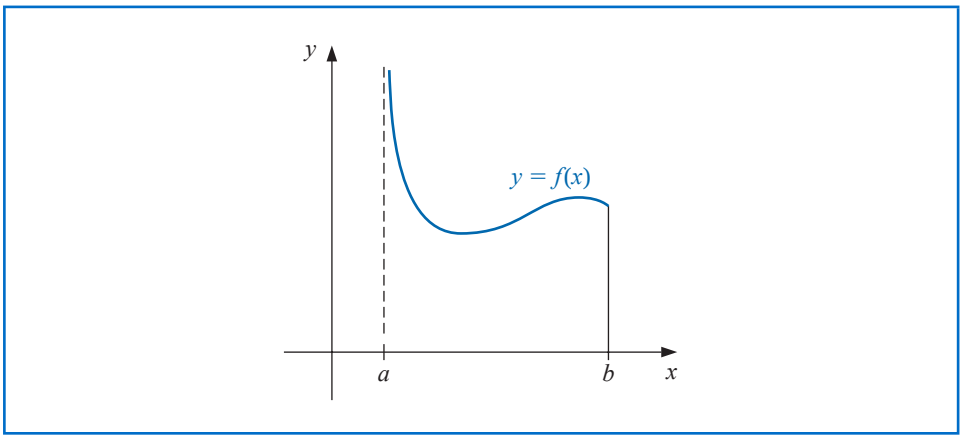
## 4.9 Improper Integrals

Improper integrals result when the notion of integration is extended either to an interval of integration on which the function is unbounded or to an interval with one or more infinite endpoints. In either circumstance, the normal rules of integral approximation must be modified.

### Left Endpoint Singularity

We will first consider the situation when the integrand is unbounded at the left endpoint of the interval of integration, as shown in Figure 4.25. In this case we say that $f$ has a **singularity** at the endpoint $a$. We will then show how other improper integrals can be reduced to problems of this form.

**Figure 4.25**




It is shown in calculus that the improper integral with a singularity at the left endpoint,

$$\int_a^b \frac{dx}{(x-a)^p},$$

converges if and only if $0 < p < 1$, and in this case, we define

$$\int_a^b \frac{1}{(x-a)^p}\,dx = \lim_{M \to a^+} \frac{(x-a)^{1-p}}{1-p}\bigg|_{x=M}^{x=b} = \frac{(b-a)^{1-p}}{1-p}.$$

**Example 1** Show that the improper integral $\displaystyle\int_0^1 \frac{1}{\sqrt{x}}\,dx$ converges but $\displaystyle\int_0^1 \frac{1}{x^2}\,dx$ diverges.

***Solution*** For the first integral we have

$$\int_0^1 \frac{1}{\sqrt{x}}\,dx = \lim_{M \to 0^+} \int_M^1 x^{-1/2}\,dx = \lim_{M \to 0^+} 2x^{1/2}\Big|_{x=M}^{x=1} = 2 - 0 = 2,$$

but the second integral

$$\int_0^1 \frac{1}{x^2}\,dx = \lim_{M \to 0^+} \int_M^1 x^{-2}\,dx = \lim_{M \to 0^+} -x^{-1}\Big|_{x=M}^{x=1}$$

is unbounded.

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If $f$ is a function that can be written in the form

$$f(x) = \frac{g(x)}{(x-a)^p},$$

where $0 < p < 1$ and $g$ is continuous on $[a, b]$, then the improper integral

$$\int_a^b f(x)\,dx$$

also exists. We will approximate this integral using the Composite Simpson's rule, provided that $g \in C^5[a, b]$. In that case, we can construct the fourth Taylor polynomial, $P_4(x)$, for $g$ about $a$,

$$P_4(x) = g(a) + g'(a)(x-a) + \frac{g''(a)}{2!}(x-a)^2 + \frac{g'''(a)}{3!}(x-a)^3 + \frac{g^{(4)}(a)}{4!}(x-a)^4,$$

and write

$$\int_a^b f(x)\,dx = \int_a^b \frac{g(x) - P_4(x)}{(x-a)^p}\,dx + \int_a^b \frac{P_4(x)}{(x-a)^p}\,dx. \tag{4.44}$$

Because $P(x)$ is a polynomial, we can exactly determine the value of

$$\int_a^b \frac{P_4(x)}{(x-a)^p}\,dx = \sum_{k=0}^{4} \int_a^b \frac{g^{(k)}(a)}{k!}(x-a)^{k-p}\,dx = \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!(k+1-p)}(b-a)^{k+1-p}. \tag{4.45}$$

This is generally the dominant portion of the approximation, especially when the Taylor polynomial $P_4(x)$ agrees closely with $g(x)$ throughout the interval $[a, b]$.

To approximate the integral of $f$, we must add to this value the approximation of

$$\int_a^b \frac{g(x) - P_4(x)}{(x-a)^p}\,dx.$$

To determine this, we first define

$$G(x) = \begin{cases} \frac{g(x)-P_4(x)}{(x-a)^p}, & \text{if } a < x \le b, \\ 0, & \text{if } x = a. \end{cases}$$

This gives us a continuous function on $[a, b]$. In fact, $0 < p < 1$ and $P_4^{(k)}(a)$ agrees with $g^{(k)}(a)$ for each $k = 0, 1, 2, 3, 4$, so we have $G \in C^4[a, b]$. This implies that the Composite Simpson's rule can be applied to approximate the integral of $G$ on $[a, b]$. Adding this approximation to the value in Eq. (4.45) gives an approximation to the improper integral of $f$ on $[a, b]$, within the accuracy of the Composite Simpson's rule approximation.

**Example 2** Use Composite Simpson's rule with $h = 0.25$ to approximate the value of the improper integral

$$\int_0^1 \frac{e^x}{\sqrt{x}}\,dx.$$

***Solution*** The fourth Taylor polynomial for $e^x$ about $x = 0$ is

$$P_4(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24},$$

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so the dominant portion of the approximation to $\int_0^1 \frac{e^x}{\sqrt{x}}\,dx$ is

$$\begin{aligned}\int_0^1 \frac{P_4(x)}{\sqrt{x}}\,dx &= \int_0^1 \left(x^{-1/2} + x^{1/2} + \frac{1}{2}x^{3/2} + \frac{1}{6}x^{5/2} + \frac{1}{24}x^{7/2}\right) dx \\ &= \lim_{M\to 0^+}\left[2x^{1/2} + \frac{2}{3}x^{3/2} + \frac{1}{5}x^{5/2} + \frac{1}{21}x^{7/2} + \frac{1}{108}x^{9/2}\right]_M^1 \\ &= 2 + \frac{2}{3} + \frac{1}{5} + \frac{1}{21} + \frac{1}{108} \approx 2.9235450.\end{aligned}$$

For the second portion of the approximation to $\int_0^1 \frac{e^x}{\sqrt{x}}\,dx$ we need to approximate $\int_0^1 G(x)\,dx$, where

$$G(x) = \begin{cases} \frac{1}{\sqrt{x}}\,(e^x - P_4(x)), & \text{if } 0 < x \le 1, \\ 0, & \text{if } x = 0. \end{cases}$$

**Table 4.13**

| $x$ | $G(x)$ |
|---|---|
| 0.00 | 0 |
| 0.25 | 0.0000170 |
| 0.50 | 0.0004013 |
| 0.75 | 0.0026026 |
| 1.00 | 0.0099485 |

Table 4.13 lists the values needed for the Composite Simpson's rule for this approximation.

Using these data and the Composite Simpson's rule gives

$$\begin{aligned}\int_0^1 G(x)\,dx &\approx \frac{0.25}{3}[0 + 4(0.0000170) + 2(0.0004013) + 4(0.0026026) + 0.0099485] \\ &= 0.0017691.\end{aligned}$$

Hence

$$\int_0^1 \frac{e^x}{\sqrt{x}}\,dx \approx 2.9235450 + 0.0017691 = 2.9253141.$$

This result is accurate to within the accuracy of the Composite Simpson's rule approximation for the function $G$. Because $|G^{(4)}(x)| < 1$ on $[0, 1]$, the error is bounded by

$$\frac{1-0}{180}(0.25)^4 = 0.0000217.$$ ■

## Right Endpoint Singularity

To approximate the improper integral with a singularity at the right endpoint, we could develop a similar technique but expand in terms of the right endpoint $b$ instead of the left endpoint $a$. Alternatively, we can make the substitution

$$z = -x, \qquad dz = -\,dx$$

to change the improper integral into one of the form

$$\int_a^b f(x)\,dx = \int_{-b}^{-a} f(-z)\,dz, \tag{4.46}$$

which has its singularity at the left endpoint. Then we can apply the left endpoint singularity technique we have already developed. (See Figure 4.26.)

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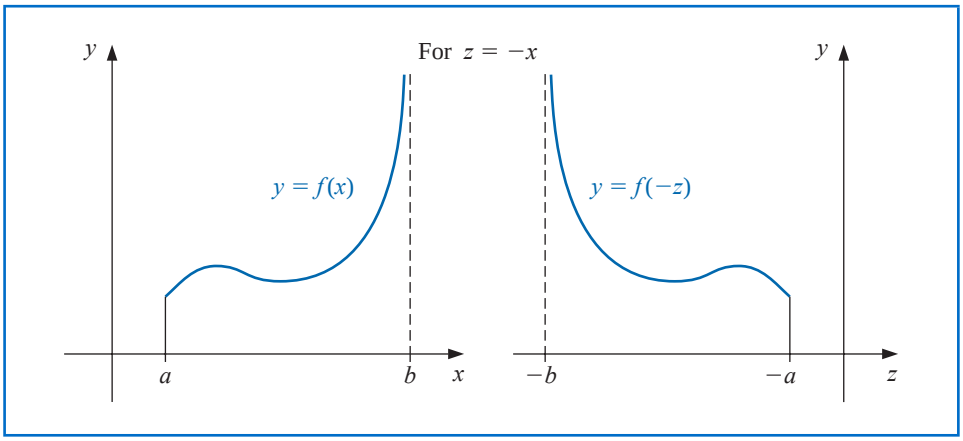
**Figure 4.26**




An improper integral with a singularity at $c$, where $a < c < b$, is treated as the sum of improper integrals with endpoint singularities since

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx.$$

## Infinite Singularity

The other type of improper integral involves infinite limits of integration. The basic integral of this type has the form

$$\int_a^\infty \frac{1}{x^p}\,dx,$$

for $p > 1$. This is converted to an integral with left endpoint singularity at 0 by making the integration substitution

$$t = x^{-1}, \quad dt = -x^{-2}\,dx, \quad \text{so} \quad dx = -x^2\,dt = -t^{-2}\,dt.$$

Then

$$\int_a^\infty \frac{1}{x^p}\,dx = \int_{1/a}^0 -\frac{t^p}{t^2}\,dt = \int_0^{1/a} \frac{1}{t^{2-p}}\,dt.$$

In a similar manner, the variable change $t = x^{-1}$ converts the improper integral $\int_a^\infty f(x)\,dx$ into one that has a left endpoint singularity at zero:

$$\int_a^\infty f(x)\,dx = \int_0^{1/a} t^{-2} f\left(\frac{1}{t}\right)\,dt. \tag{4.47}$$

It can now be approximated using a quadrature formula of the type described earlier.

**Example 3** Approximate the value of the improper integral

$$I = \int_1^\infty x^{-3/2} \sin\frac{1}{x}\,dx.$$

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***Solution*** We first make the variable change $t = x^{-1}$, which converts the infinite singularity into one with a left endpoint singularity. Then

$$dt = -x^{-2}\,dx, \quad \text{so} \quad dx = -x^2\,dt = -\frac{1}{t^2}\,dt,$$

and

$$I = \int_{x=1}^{x=\infty} x^{-3/2} \sin\frac{1}{x}\,dx = \int_{t=1}^{t=0} \left(\frac{1}{t}\right)^{-3/2} \sin t \left(-\frac{1}{t^2}\,dt\right) = \int_0^1 t^{-1/2} \sin t\,dt.$$

The fourth Taylor polynomial, $P_4(t)$, for $\sin t$ about 0 is

$$P_4(t) = t - \frac{1}{6}t^3,$$

so

$$G(t) = \begin{cases} \dfrac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}, & \text{if } 0 < t \le 1 \\ 0, & \text{if } t = 0 \end{cases}$$

is in $C^4[0, 1]$, and we have

$$\begin{aligned} I &= \int_0^1 t^{-1/2}\left(t - \frac{1}{6}t^3\right) dt + \int_0^1 \frac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}\,dt \\ &= \left[\frac{2}{3}t^{3/2} - \frac{1}{21}t^{7/2}\right]_0^1 + \int_0^1 \frac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}\,dt \\ &= 0.61904761 + \int_0^1 \frac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}\,dt. \end{aligned}$$

The result from the Composite Simpson's rule with $n = 16$ for the remaining integral is 0.0014890097. This gives a final approximation of

$$I = 0.0014890097 + 0.61904761 = 0.62053661,$$

which is accurate to within $4.0 \times 10^{-8}$. ■

## EXERCISE SET 4.9

**1.** Use Simpson's Composite rule and the given values of $n$ to approximate the following improper integrals.

**a.** $\displaystyle\int_0^1 x^{-1/4} \sin x\,dx, \quad n = 4$

**b.** $\displaystyle\int_0^1 \frac{e^{2x}}{\sqrt[5]{x^2}}\,dx, \quad n = 6$

**c.** $\displaystyle\int_1^2 \frac{\ln x}{(x-1)^{1/5}}\,dx, \quad n = 8$

**d.** $\displaystyle\int_0^1 \frac{\cos 2x}{x^{1/3}}\,dx, \quad n = 6$

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**2.** Use the Composite Simpson's rule and the given values of $n$ to approximate the following improper integrals.

**a.** $\displaystyle\int_0^1 \frac{e^{-x}}{\sqrt{1-x}}\,dx, \quad n = 6$

**b.** $\displaystyle\int_0^2 \frac{xe^x}{\sqrt[3]{(x-1)^2}}\,dx, \quad n = 8$

**3.** Use the transformation $t = x^{-1}$ and then the Composite Simpson's rule and the given values of $n$ to approximate the following improper integrals.

**a.** $\displaystyle\int_1^\infty \frac{1}{x^2+9}\,dx, \quad n = 4$

**b.** $\displaystyle\int_1^\infty \frac{1}{1+x^4}\,dx, \quad n = 4$

**c.** $\displaystyle\int_1^\infty \frac{\cos x}{x^3}\,dx, \quad n = 6$

**d.** $\displaystyle\int_1^\infty x^{-4}\sin x\,dx, \quad n = 6$

**4.** The improper integral $\int_0^\infty f(x)\,dx$ cannot be converted into an integral with finite limits using the substitution $t = 1/x$ because the limit at zero becomes infinite. The problem is resolved by first writing $\int_0^\infty f(x)\,dx = \int_0^1 f(x)\,dx + \int_1^\infty f(x)\,dx$. Apply this technique to approximate the following improper integrals to within $10^{-6}$.

**a.** $\displaystyle\int_0^\infty \frac{1}{1+x^4}\,dx$

**b.** $\displaystyle\int_0^\infty \frac{1}{(1+x^2)^3}\,dx$

**5.** Suppose a body of mass $m$ is traveling vertically upward starting at the surface of the earth. If all resistance except gravity is neglected, the escape velocity $v$ is given by

$$v^2 = 2gR\int_1^\infty z^{-2}\,dz, \quad \text{where } z = \frac{x}{R},$$

$R = 3960$ miles is the radius of the earth, and $g = 0.00609$ mi/s$^2$ is the force of gravity at the earth's surface. Approximate the escape velocity $v$.

**6.** The Laguerre polynomials $\{L_0(x), L_1(x)\ldots\}$ form an orthogonal set on $[0,\infty)$ and satisfy $\int_0^\infty e^{-x}L_i(x)L_j(x)\,dx = 0$, for $i \neq j$. (See Section 8.2.) The polynomial $L_n(x)$ has $n$ distinct zeros $x_1, x_2, \ldots, x_n$ in $[0,\infty)$. Let

$$c_{n,i} = \int_0^\infty e^{-x}\prod_{\substack{j=1\\ j\neq i}}^{n}\frac{x-x_j}{x_i-x_j}\,dx.$$

Show that the quadrature formula

$$\int_0^\infty f(x)e^{-x}\,dx = \sum_{i=1}^{n} c_{n,i}f(x_i)$$

has degree of precision $2n-1$. (Hint: Follow the steps in the proof of Theorem 4.7.)

**7.** The Laguerre polynomials $L_0(x) = 1$, $L_1(x) = 1-x$, $L_2(x) = x^2-4x+2$, and $L_3(x) = -x^3+9x^2-18x+6$ are derived in Exercise 11 of Section 8.2. As shown in Exercise 6, these polynomials are useful in approximating integrals of the form

$$\int_0^\infty e^{-x}f(x)\,dx = 0.$$

**a.** Derive the quadrature formula using $n = 2$ and the zeros of $L_2(x)$.

**b.** Derive the quadrature formula using $n = 3$ and the zeros of $L_3(x)$.

**8.** Use the quadrature formulas derived in Exercise 7 to approximate the integral

$$\int_0^\infty \sqrt{x}e^{-x}\,dx.$$

**9.** Use the quadrature formulas derived in Exercise 7 to approximate the integral

$$\int_{-\infty}^\infty \frac{1}{1+x^2}\,dx.$$

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## 4.10 Survey of Methods and Software

In this chapter we considered approximating integrals of functions of one, two, or three variables, and approximating the derivatives of a function of a single real variable.

The Midpoint rule, Trapezoidal rule, and Simpson's rule were studied to introduce the techniques and error analysis of quadrature methods. Composite Simpson's rule is easy to use and produces accurate approximations unless the function oscillates in a subinterval of the interval of integration. Adaptive quadrature can be used if the function is suspected of oscillatory behavior. To minimize the number of nodes while maintaining accuracy, we used Gaussian quadrature. Romberg integration was introduced to take advantage of the easily applied Composite Trapezoidal rule and extrapolation.

Most software for integrating a function of a single real variable is based either on the adaptive approach or extremely accurate Gaussian formulas. Cautious Romberg integration is an adaptive technique that includes a check to make sure that the integrand is smoothly behaved over subintervals of the integral of integration. This method has been successfully used in software libraries. Multiple integrals are generally approximated by extending good adaptive methods to higher dimensions. Gaussian-type quadrature is also recommended to decrease the number of function evaluations.

The main routines in both the IMSL and NAG Libraries are based on *QUADPACK: A Subroutine Package for Automatic Integration* by R. Piessens, E. de Doncker-Kapenga, C. W. Uberhuber, and D. K. Kahaner published by Springer-Verlag in 1983 [PDUK].

The IMSL Library contains an adaptive integration scheme based on the 21-point Gaussian-Kronrod rule using the 10-point Gaussian rule for error estimation. The Gaussian rule uses the ten points $x_1, \ldots, x_{10}$ and weights $w_1, \ldots, w_{10}$ to give the quadrature formula $\sum_{i=1}^{10} w_i f(x_i)$ to approximate $\int_a^b f(x)\,dx$. The additional points $x_{11}, \ldots, x_{21}$, and the new weights $v_1, \ldots, v_{21}$, are then used in the Kronrod formula $\sum_{i=1}^{21} v_i f(x_i)$. The results of the two formulas are compared to eliminate error. The advantage in using $x_1, \ldots, x_{10}$ in each formula is that $f$ needs to be evaluated only at 21 points. If independent 10- and 21-point Gaussian rules were used, 31 function evaluations would be needed. This procedure permits endpoint singularities in the integrand.

Other IMSL subroutines allow for endpoint singularities, user-specified singularities, and infinite intervals of integration. In addition, there are routines for applying Gauss-Kronrod rules to integrate a function of two variables, and a routine to use Gaussian quadrature to integrate a function of $n$ variables over $n$ intervals of the form $[a_i, b_i]$.

The NAG Library includes a routine to compute the integral of $f$ over the interval $[a, b]$ using an adaptive method based on Gaussian Quadrature using Gauss 10-point and Kronrod 21-point rules. It also has a routine to approximate an integral using a family of Gaussian-type formulas based on 1, 3, 5, 7, 15, 31, 63, 127, and 255 nodes. These interlacing high-precision rules are due to Patterson [Pat] and are used in an adaptive manner. NAG includes many other subroutines for approximating integrals.

MATLAB has a routine to approximate a definite integral using an adaptive Simpson's rule, and another to approximate the definite integral using an adaptive eight-panel Newton-Cotes rule.

Although numerical differentiation is unstable, derivative approximation formulas are needed for solving differential equations. The NAG Library includes a subroutine for the numerical differentiation of a function of one real variable with differentiation to the fourteenth derivative being possible. IMSL has a function that uses an adaptive change in step size for finite differences to approximate the first, second, or third, derivative of $f$ at $x$ to within a given tolerance. IMSL also includes a subroutine to compute the derivatives of a function defined on a set of points using quadratic interpolation. Both packages allow the

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differentiation and integration of interpolatory cubic splines constructed by the subroutines mentioned in Section 3.5.

For further reading on numerical integration we recommend the books by Engels [E] and by Davis and Rabinowitz [DR]. For more information on Gaussian quadrature see Stroud and Secrest [StS]. Books on multiple integrals include those by Stroud [Stro] and by Sloan and Joe [SJ].

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